Key elements in NEMO to quantitative nano-scale carrier transport analysis in semiconductors

Gerhard Klimeck

Jet Propulsion Laboratory, California Institute of Technology

gekco@jpl.nasa.gov

(818) 354 2182

http://hpc.jpl.nasa.gov/PEP/gekco

This research was carried out in part by at the Jet Propulsion Laboratory, California Institute of Technology under a contract with the National Aeronautics and Space Administration.

Funding by NRO, ARDA, ONR, NASA, JPL

Thanks to:
NEMO Core Team Members

NEMO 1-D

Roger Lake, Texas Instruments / UC Riverside

R. Chris Bowen, Texas Instruments / JPL / Texas Instruments

Tim Boykin, U Alabama in Huntsville

Dan Blanks, Texas Instruments

William R. Frensley, UT Dallas

NEMO 3-D / Synthesis

Fabiano Oyafuso, JPL

Seungwon Lee, JPL

Paul von Allmen, JPL

Olga Lazarenkova, JPL

R. Chris Bowen, JPL

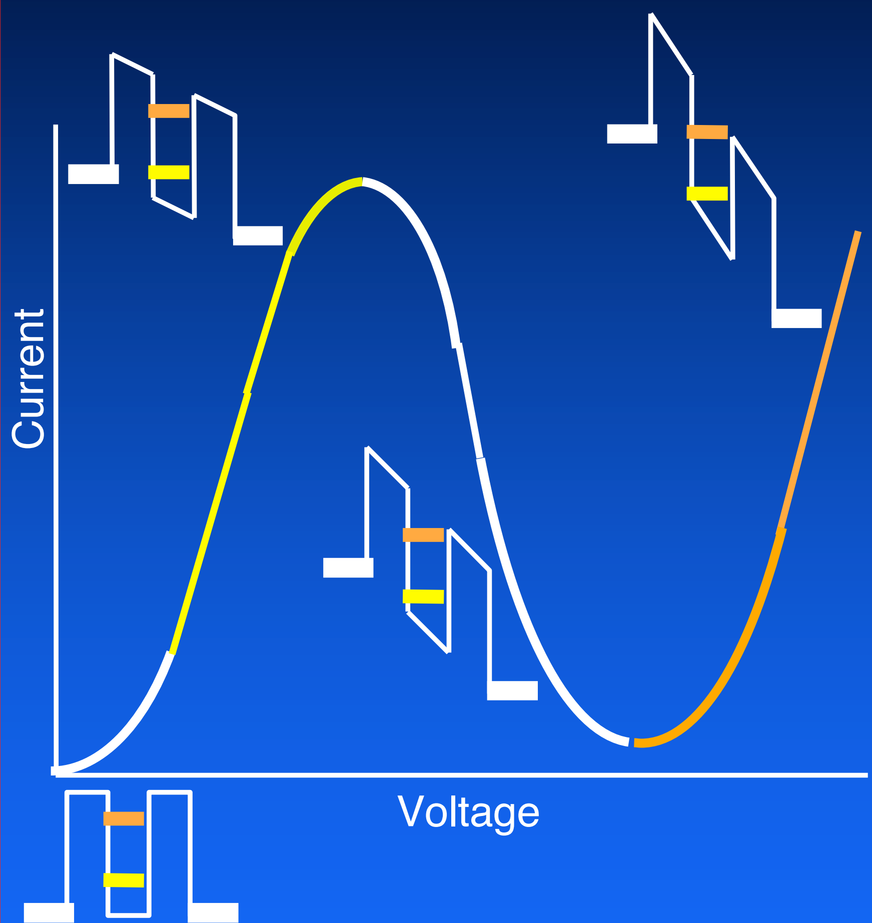
Thomas A. Cwik, JPL

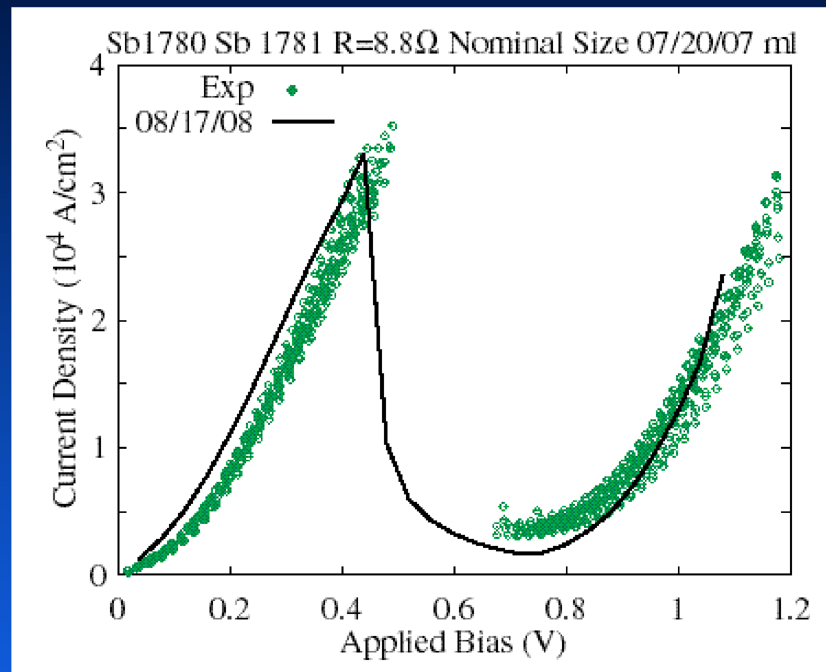
Funding by NRO, ARDA, ONR, NASA, JPL

Outline:
Key Elements to NEMO

- **NEMO Goal:**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- **Anticipated / Expected:**
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- **Unexpected / Breakthroughs:**
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, complex band warping, indirect gaps
- **Putting it all together**
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**

Resonant Tunneling Diode





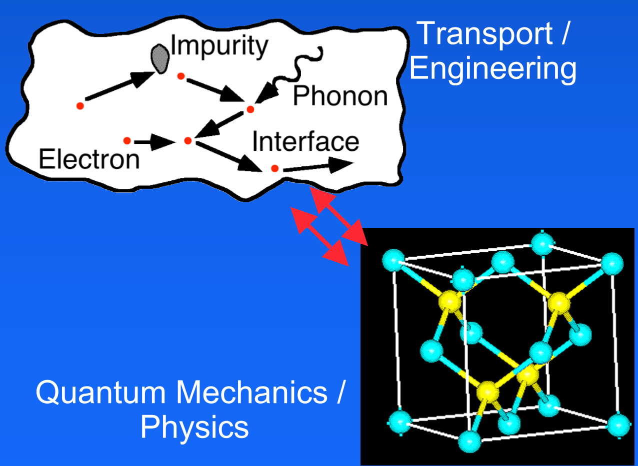
12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

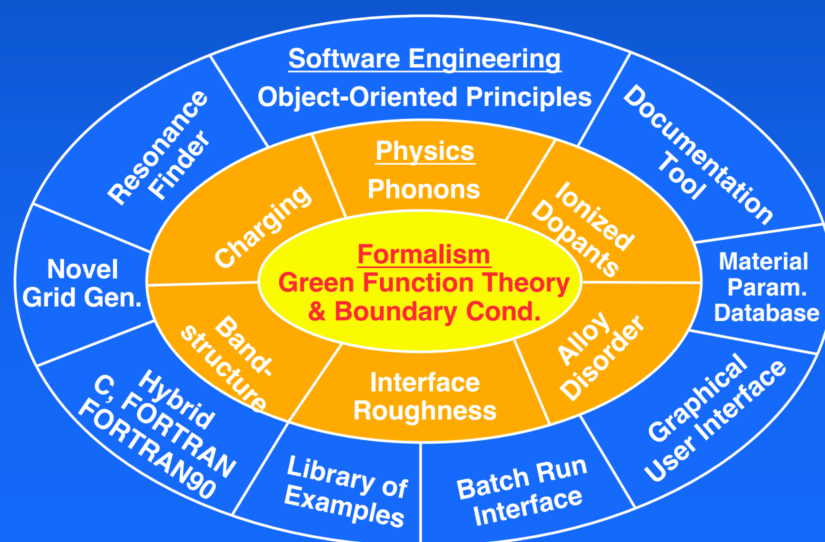
50nm	1e18	InGaAs
7 ml	nid	InGaAs
7 ml	nid	AlAs
20 ml	nid	InGaAs
7 ml	nid	AlAs
7 ml	nid	InGaAs
50 nm	1e18	InGaAs

Conduction band diagrams for different voltages and the resulting current flow.

NEMO:
A User-friendly Quantum Device Design Tool

- NEMO 1-D was developed under a NSA/NRO contract to Texas Instruments and Raytheon from ‘93-’98 (>50,000 person hours, 250,000 lines of code).
- NEMO 1-D maintained and NEMO 3-D developed at JPL ‘98-’02 (>12000 person hours) under NASA funding. Since ‘02 NSA and ONR funding.
- NEMO is THE state-of-the-art quantum device design tool.
  - First target: transport through resonant tunneling diodes (high speed electronics).
  - Second target: electronic structure in realistically large nano devices (detectors).
  - Newly set target: qbit device simulation.
- Bridges the gap between device engineering and quantum physics.
- Based on Non-Equilibrium Green function formalism NEGF - Datta, Lake, and Klimeck.
- Used at Intel, Motorola, HP, Texas Instruments, and >10 Universities.

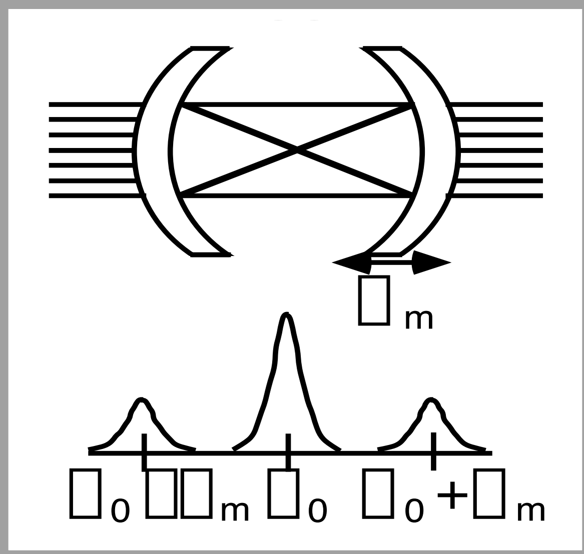


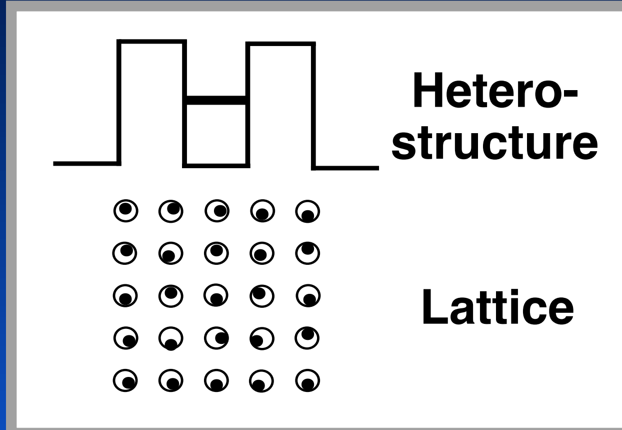


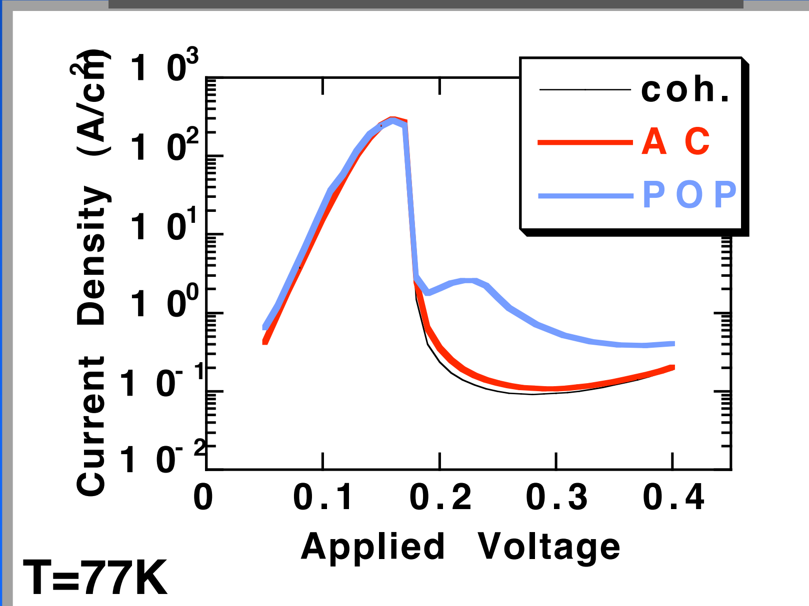
Outline:
Key Elements to NEMO

- **NEMO Goal:**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- **Anticipated / Expected:**
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- **Unexpected / Breakthroughs:**
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, complex band warping, indirect gaps
- **Putting it all together**
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**

Electron-Phonon Interactions
Coupled Resonators



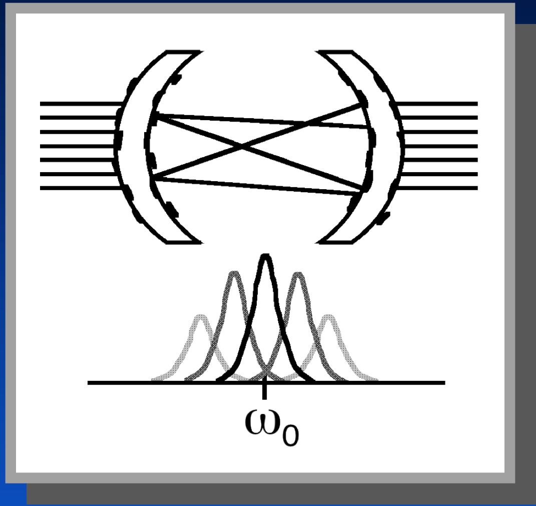


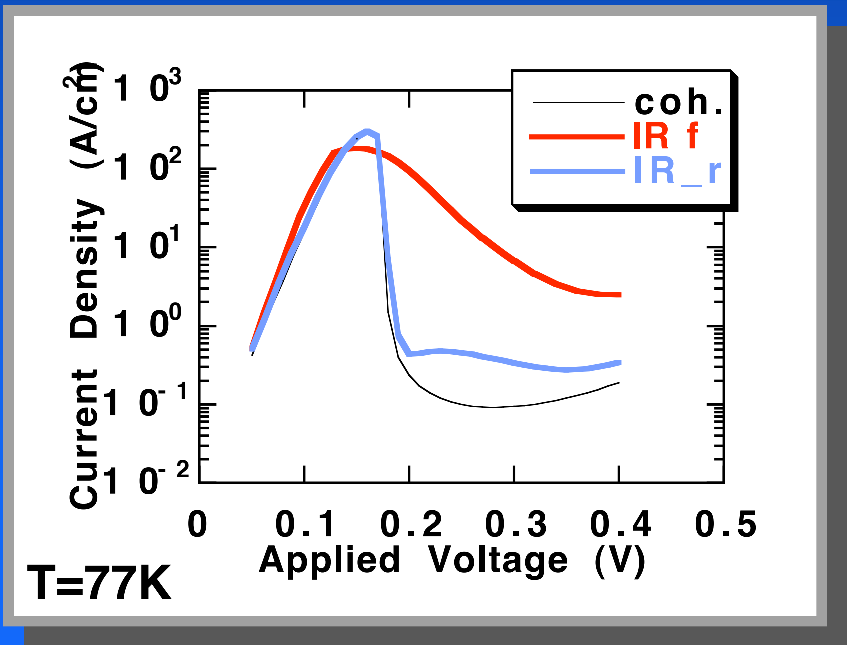


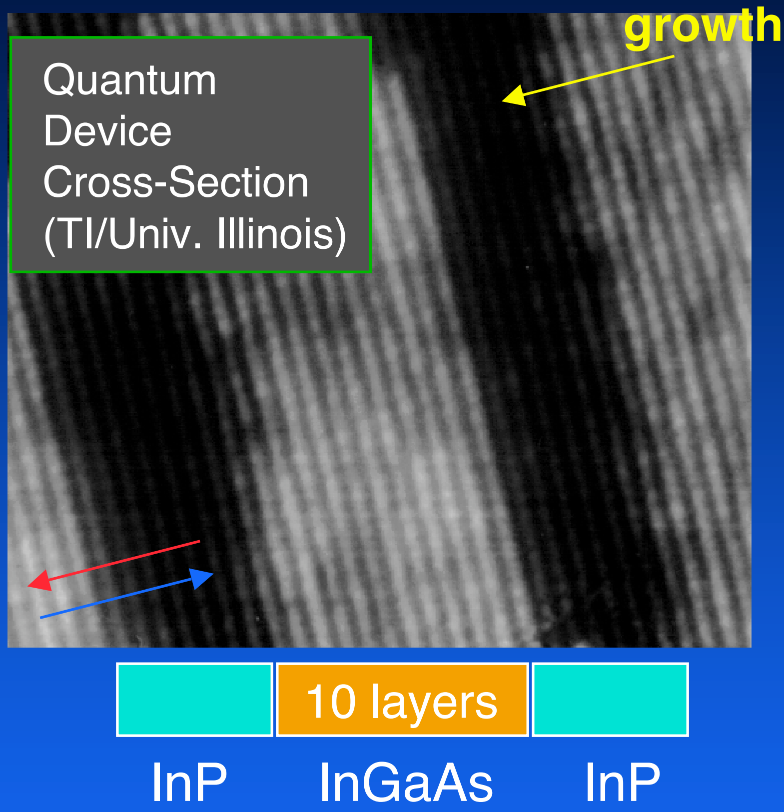
Self-consistent Born
(infinite sequential scattering)
treatment of
acoustic phonon-scattering

Single sequential scattering
treatment of
polar optical phonon scattering

Interface Roughness Scattering

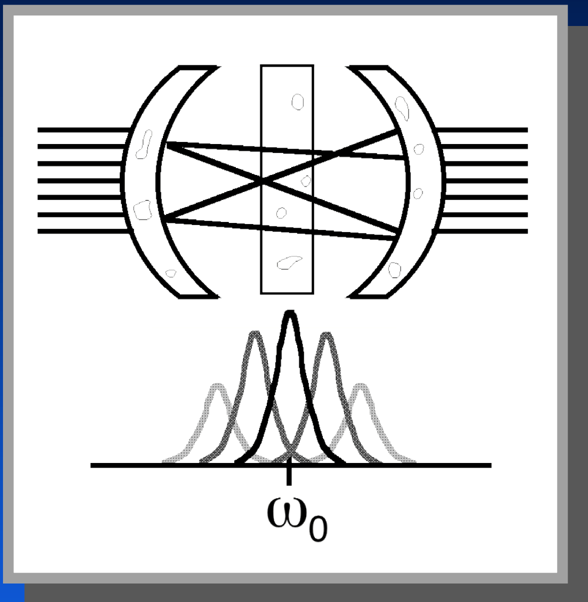




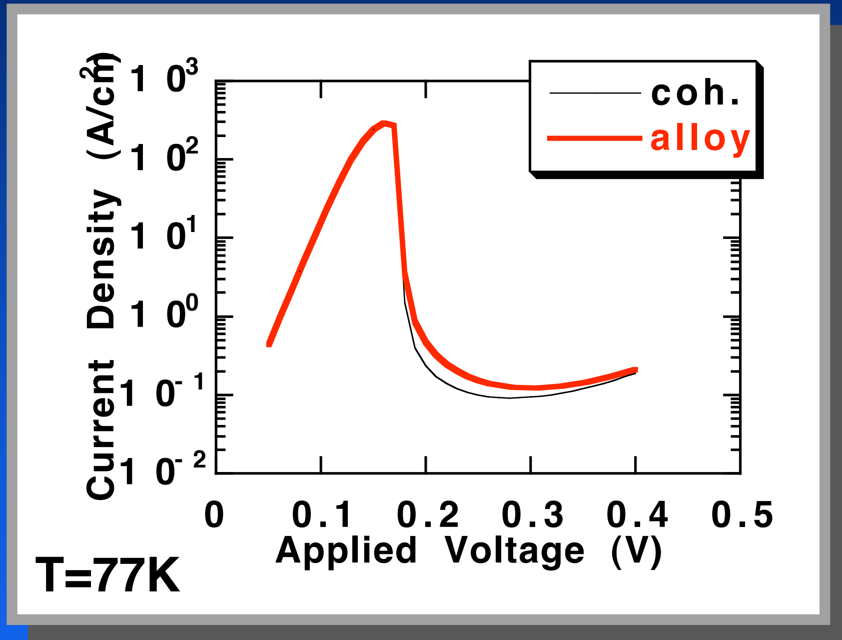


Self-consistent Born (infinite sequential scattering) treatment of IR-scattering

Alloy (Disorder) Scattering

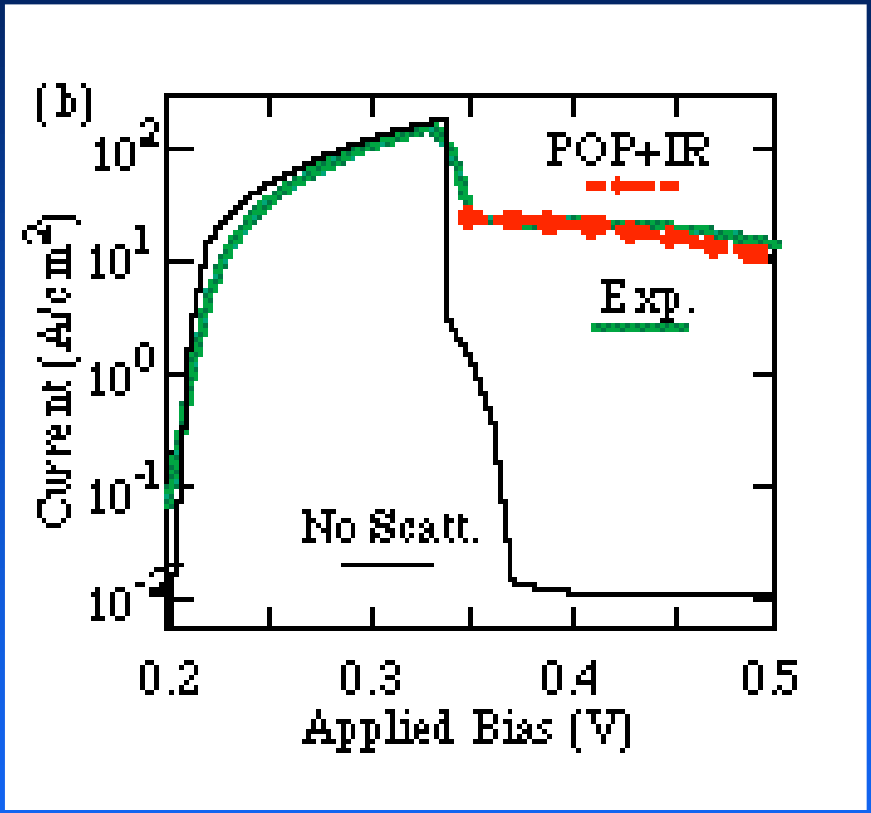


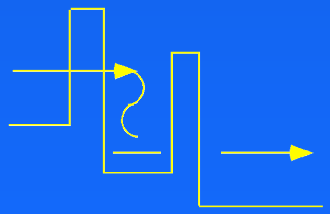
Disorder in the mirrors or the gain medium will spread out the resonator spectrum



Self-consistent Born (infinite sequential scattering) treatment of alloy-scattering

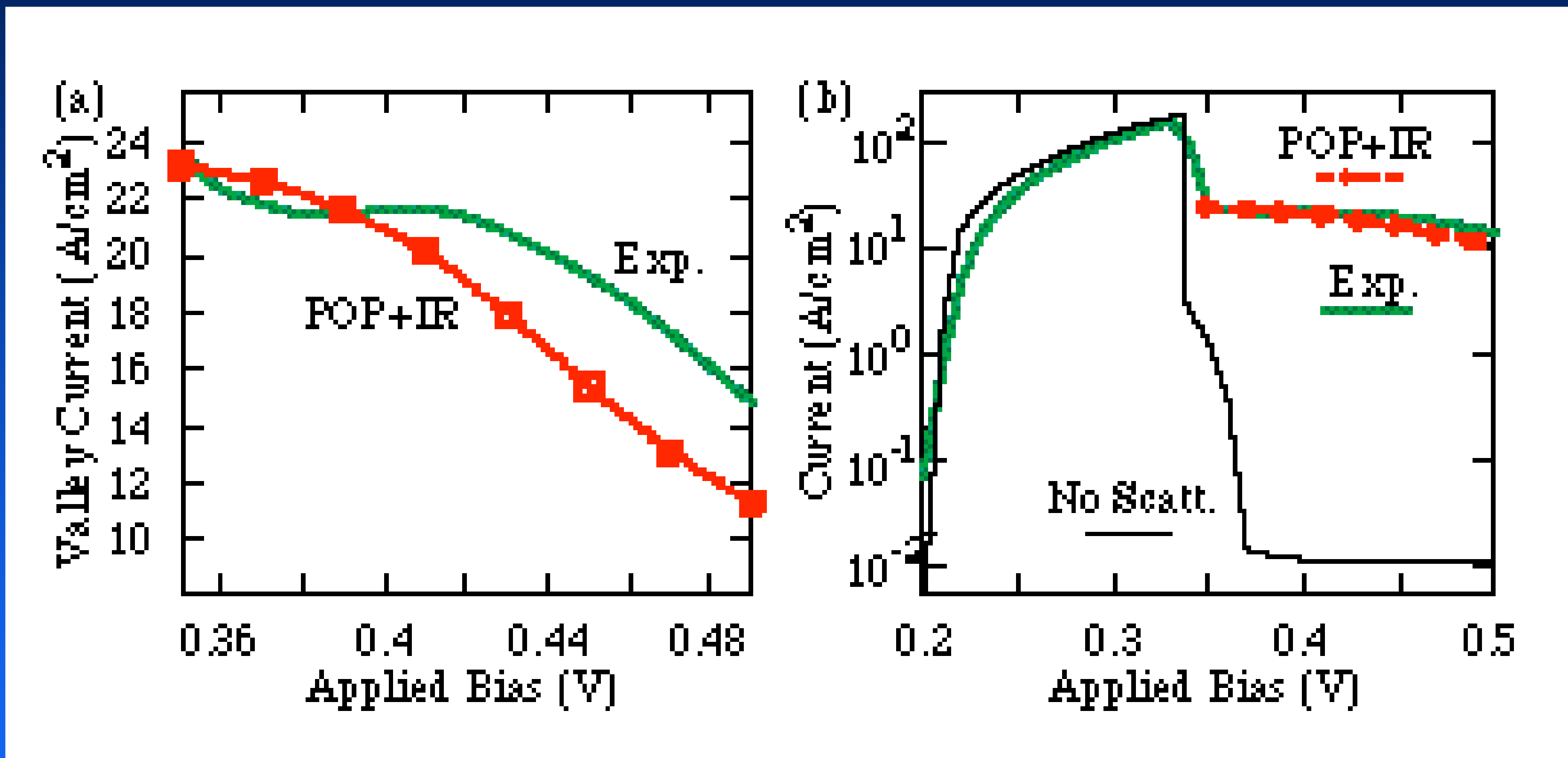
Tow Temperature: Polar Optical Phonon and Interface Roughness Scattering

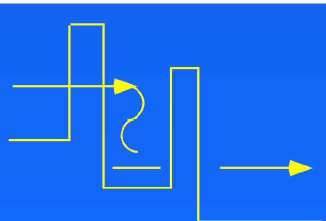




scattering raises valley current
by several orders of magnitude

Tow Temperature: Polar Optical Phonon and Interface Roughness Scattering





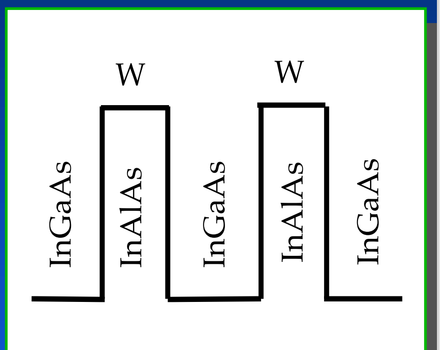
scattering raises valley current by several orders of magnitude

Outline:
Key Elements to NEMO

- **NEMO Goal:**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- **Anticipated / Expected:**
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- **Unexpected / Breakthroughs:**
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, complex band warping, indirect gaps
- **Putting it all together**
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**

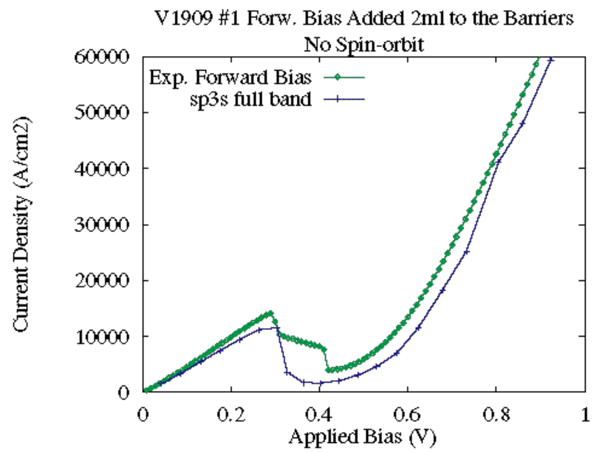
Charge Accumulation/Depletion

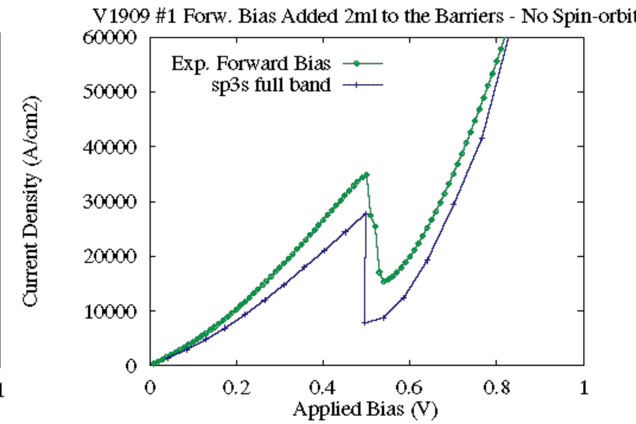
Vary Well Width



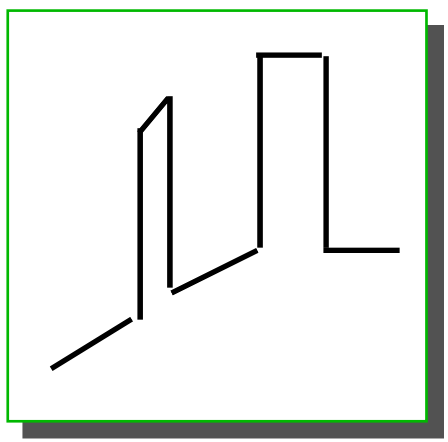
asymmetric device: 35/47/47 A [4]

Asymmetric Device

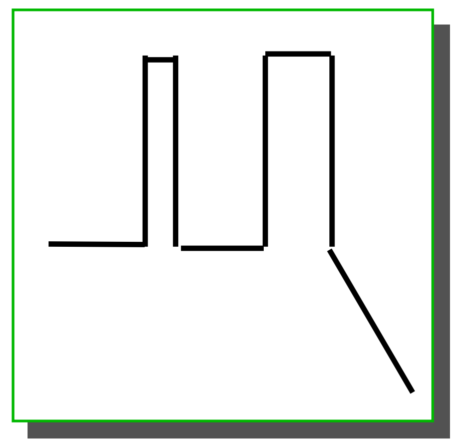




Reverse Bias



Forward Bias



Symmetric RTD's: Charge Self-Consistency Still Important!

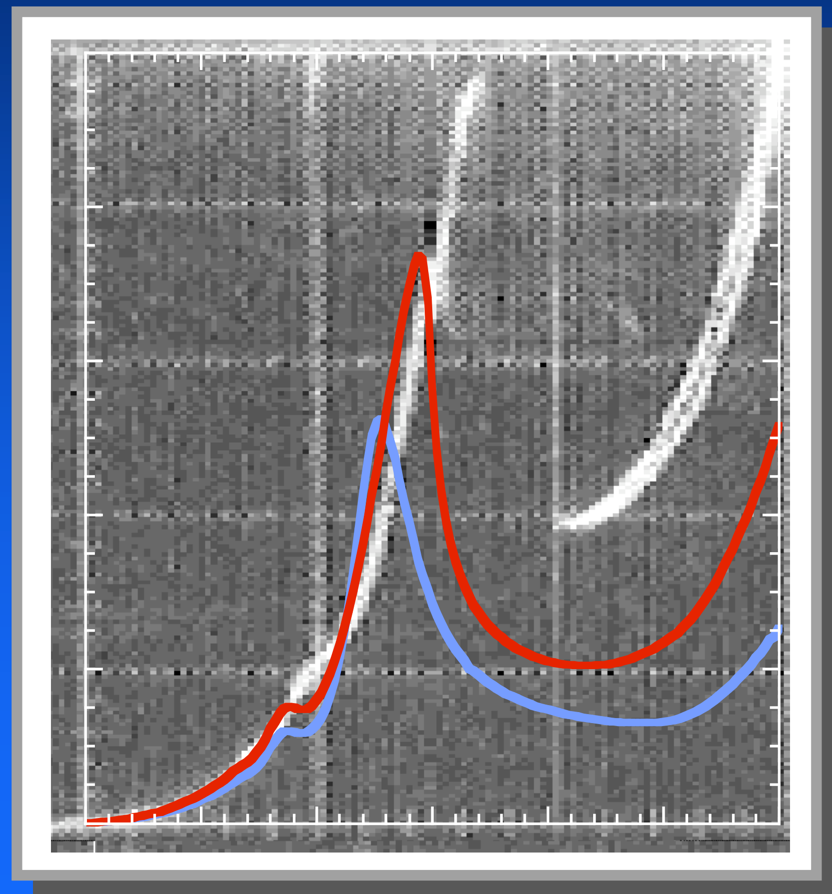
Outline: Key Elements to NEMO

- •NEMO Goal:
  - •Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - •Faster simulation than experimental turn-around (1 week).
- •Anticipated / Expected:
  - •Scattering - origin of the valley current.
  - •Charge self-consistency - position of voltage peak.
- •Unexpected / Breakthroughs:
  - •Treatment of extended contact regions
  - •Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - •Non-parabolicity, complex band warping, indirect gaps
- •Putting it all together
  - •NEMO - testmatrix
  - •The next step: automated analysis and SYNTHESIS

•Unexpected / Breakthroughs:

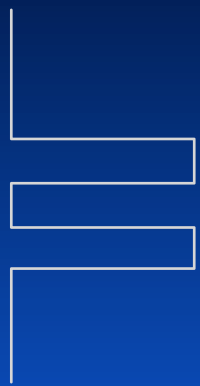
•Treatment of extended contact regions

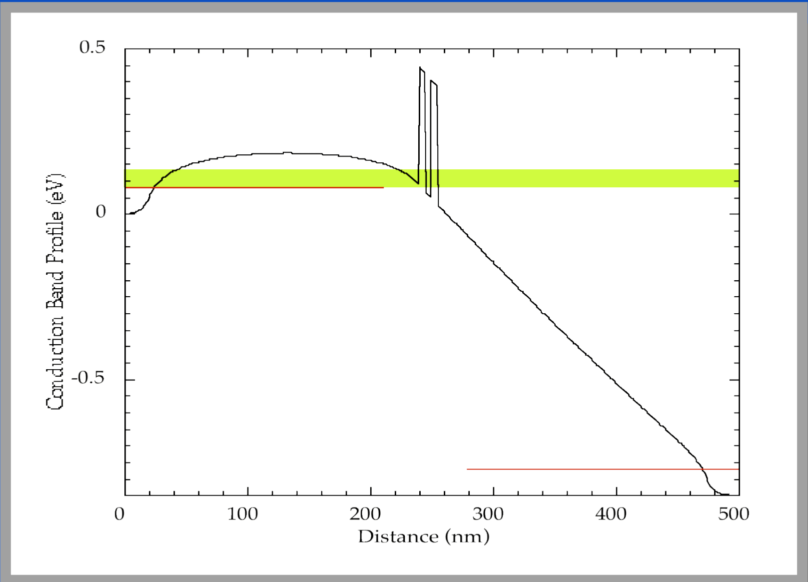
Thomas-Fermi
Hartree

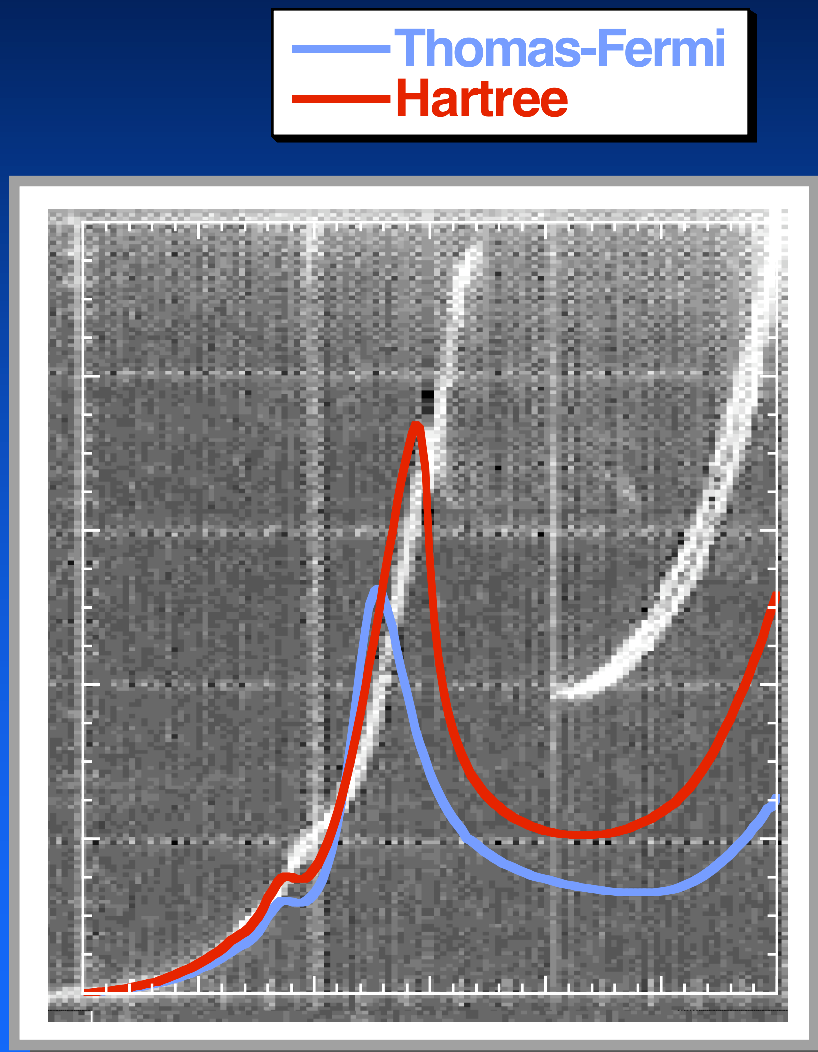


Modeling of a Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD

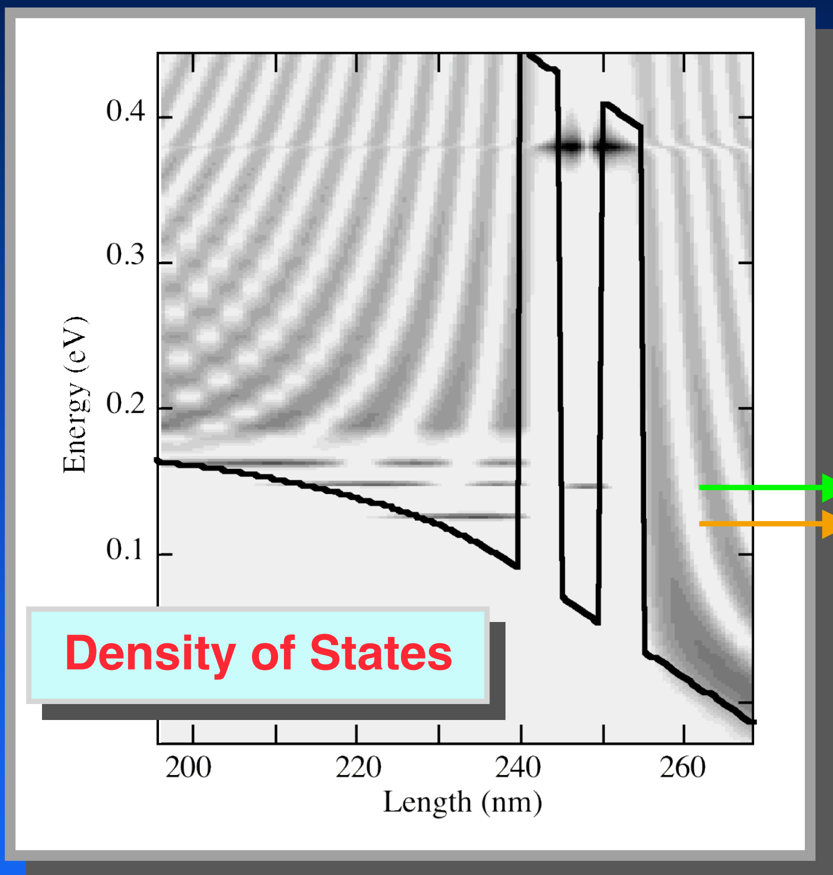
20 nm GaAs $N_D = 2\ 10^{18}\ cm^{-3}$
200 nm GaAs $N_D = 2\ 10^{15}\ cm^{-3}$
18 nm GaAs
5 nm $Al_{0.4}Ga_{0.6}As$
5 nm GaAs
5 nm $Al_{0.4}Ga_{0.6}As$
18 nm GaAs
200 nm GaAs $N_D = 2\ 10^{15}\ cm^{-3}$
20 nm GaAs $N_D = 2\ 10^{18}\ cm^{-3}$

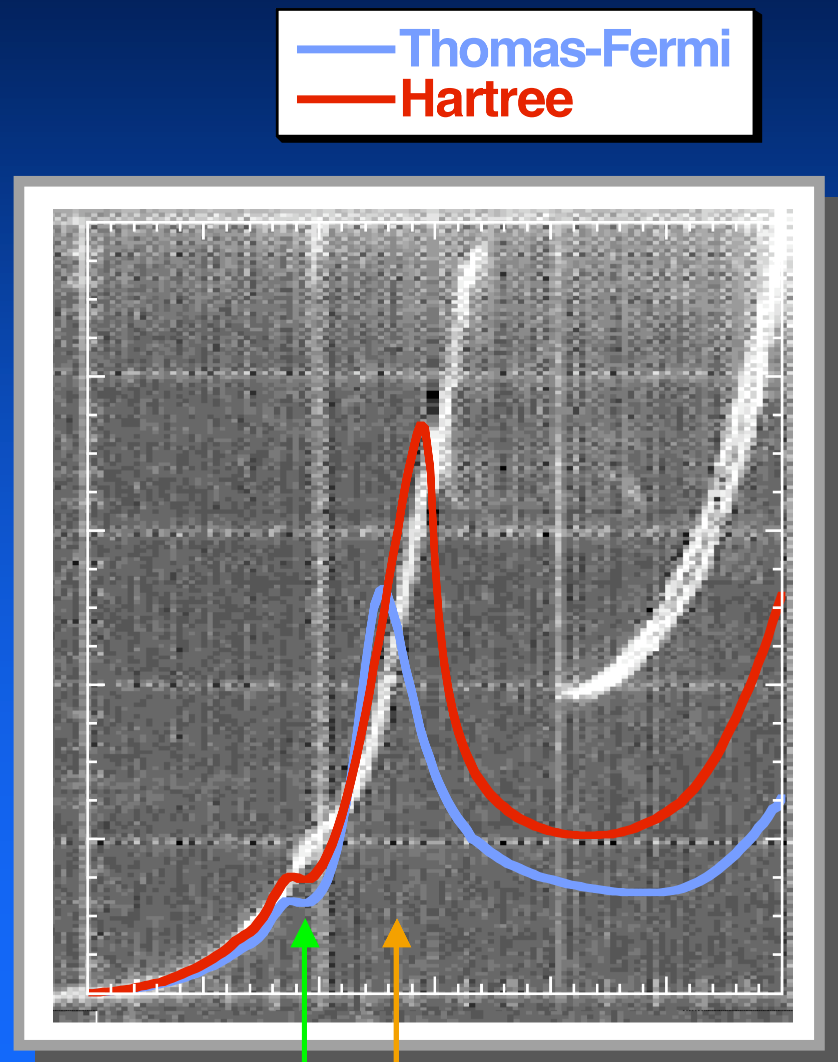






Modeling of a Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD

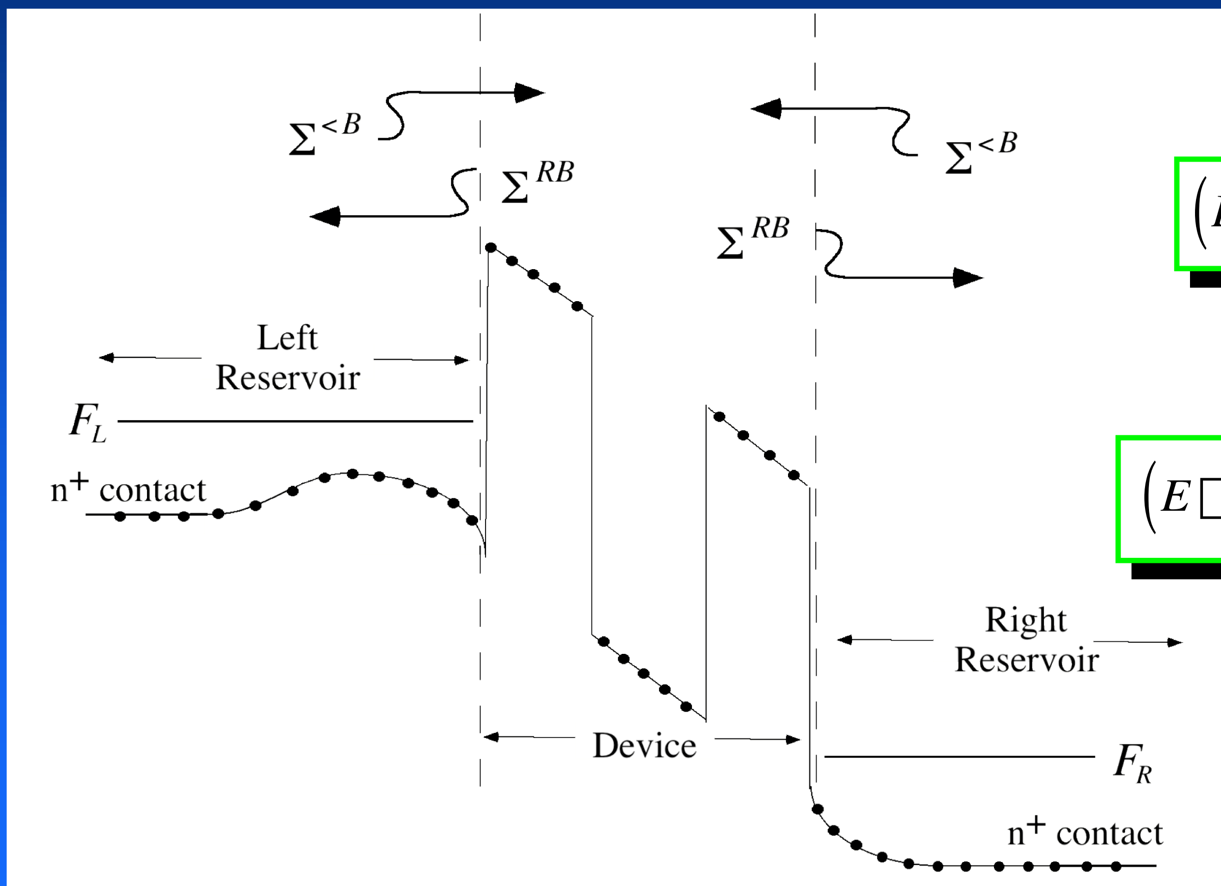




Carrier Injection from:
- **Emitter bound states**
- **Continuum states.**

Generalized Boundary Conditions: Boundaries as a Scattering Problem

- Left and right regions are treated as reservoirs.
- Quantum structure of reservoirs is included exactly.



Dynamics

$$\left(E - H_0 - \Sigma^{RB}\right) G^R = 1$$

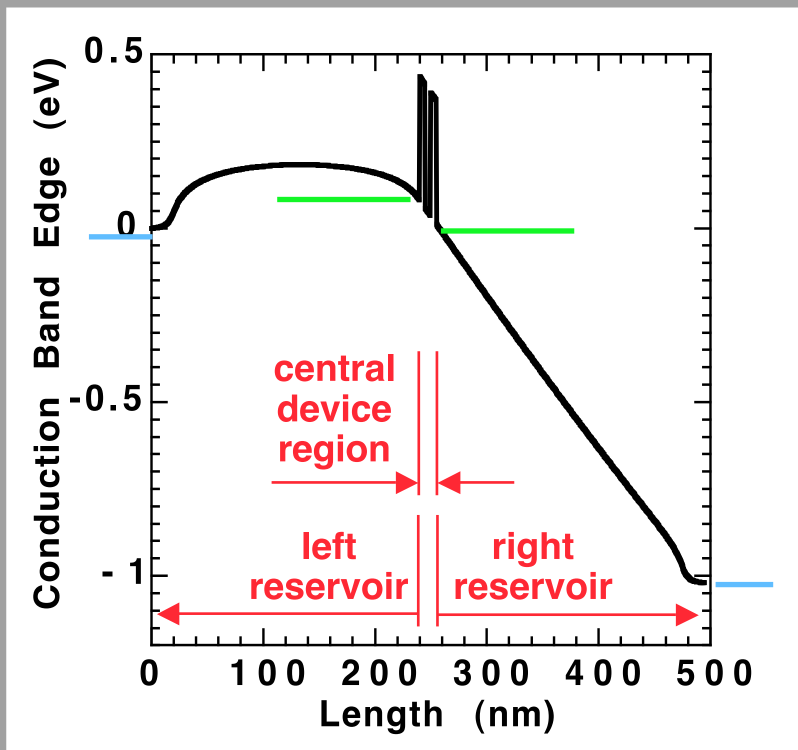
$$\left(E - H_0 - \Sigma^{RB}\right) G^< = \Sigma^{<B} G^A$$

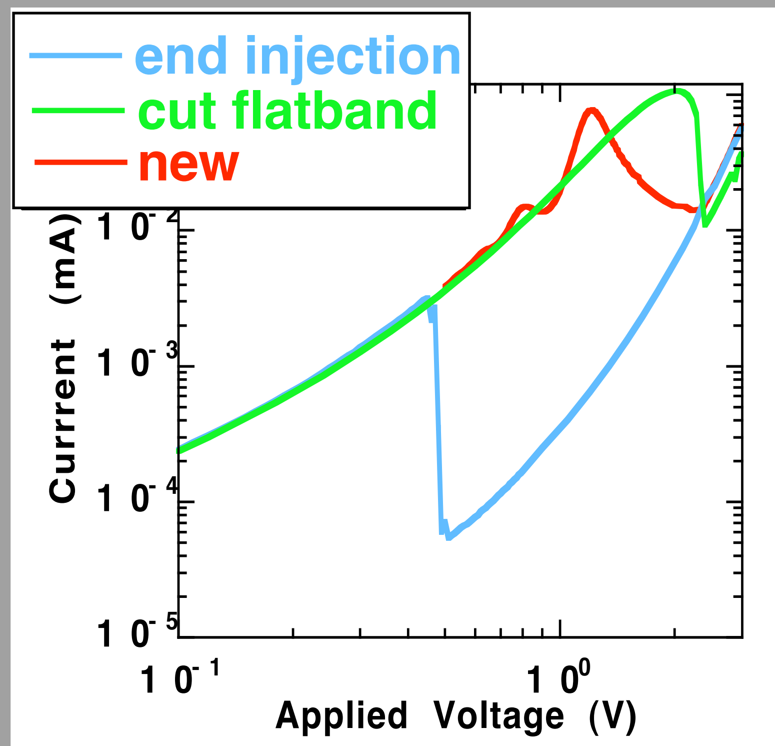
Kinetics

Treatment of the Electron Reservoirs

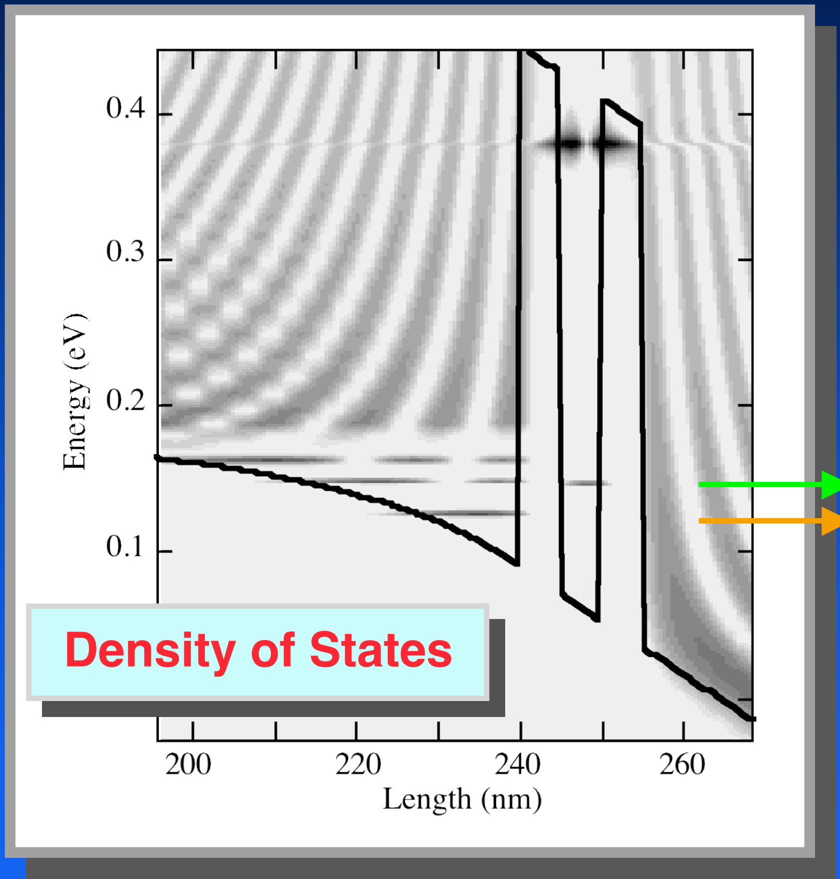
Typical Methods:
- Injection from reservoirs with flat bands

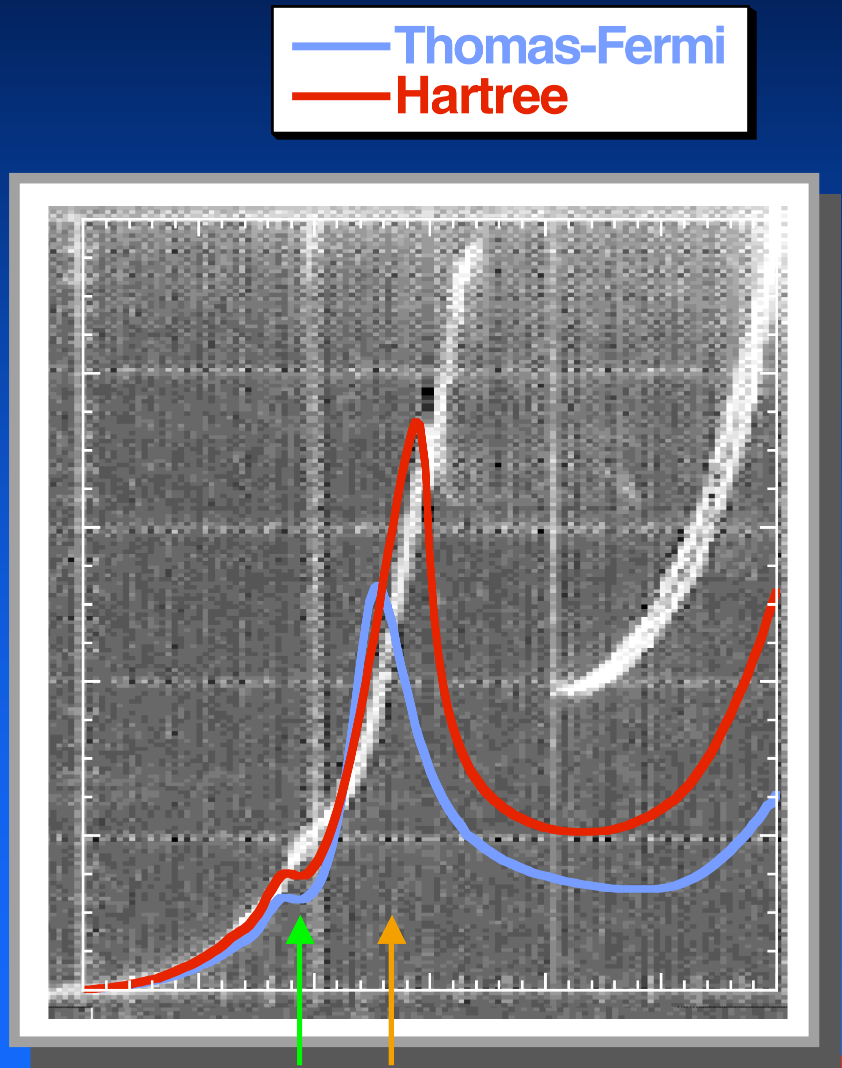
New Method:
- Injection of carriers from reservoirs with bent bands
- Modified densities of states





Modeling of a Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD





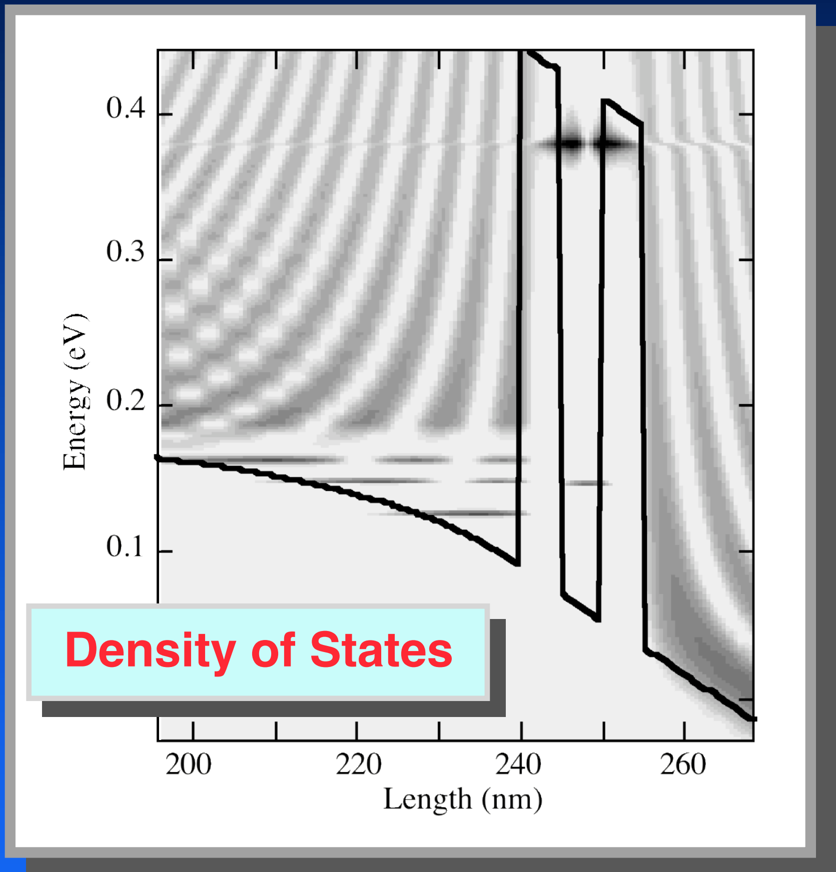
Where does the valley current current come from?

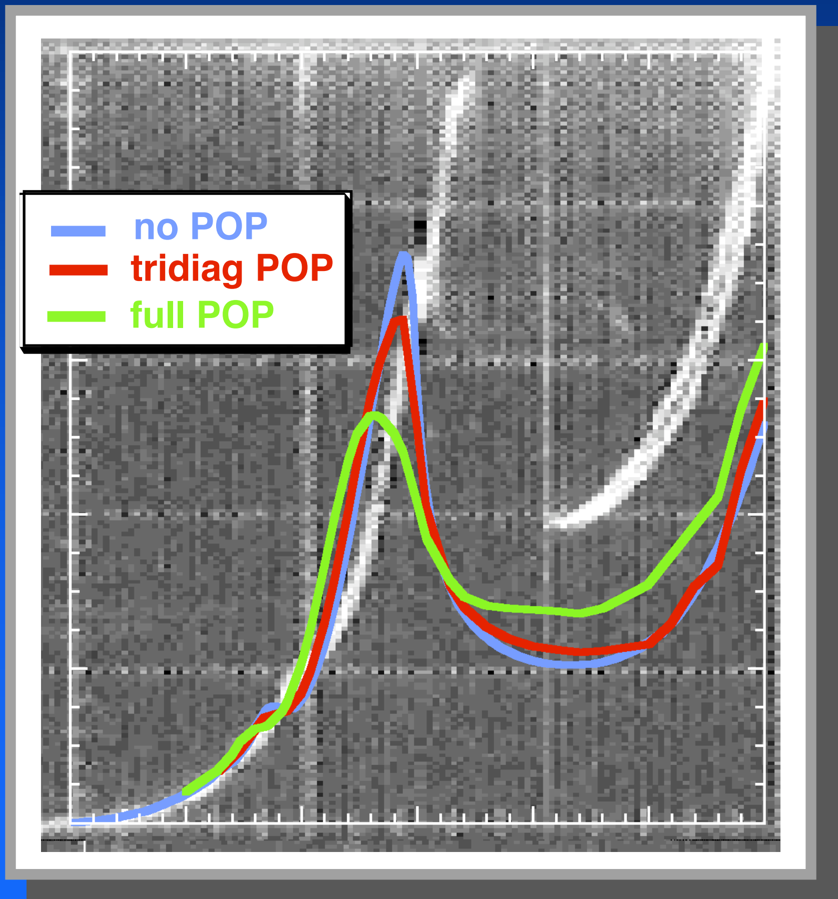
Self-consistency helps - not enough

Modeling of a Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD

Single band with scattering

POP = Polar Optical Phonons





Where does the valley current current come from?
POP is the only efffective scattering mechanism - not enough

Modeling of a Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD

Single band with scattering

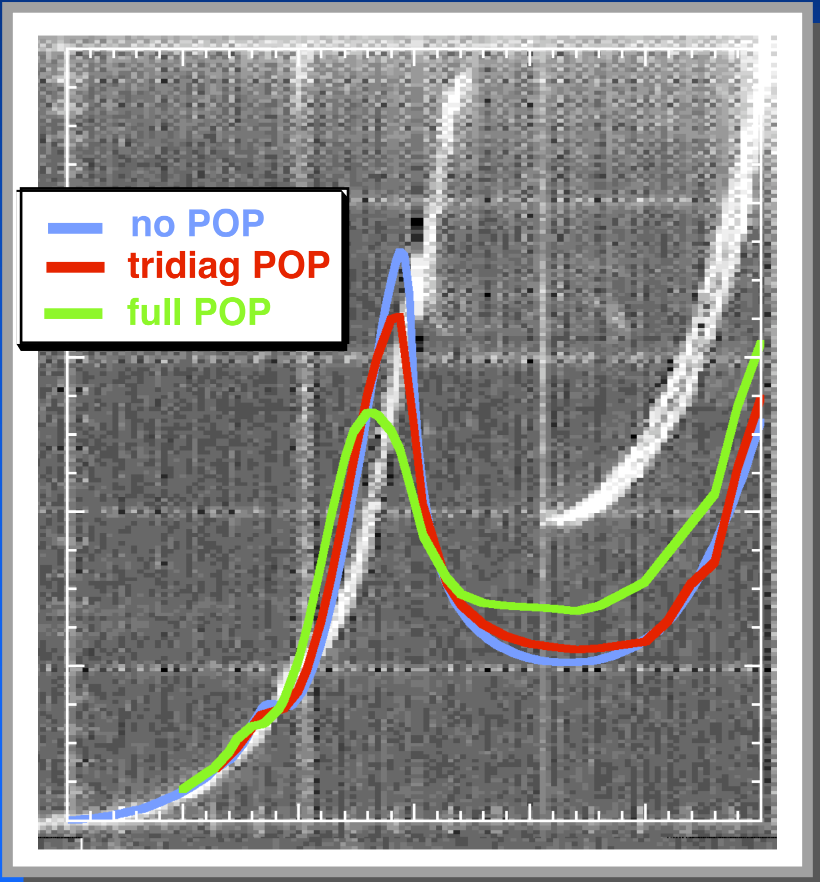
POP = Polar Optical Phonons

Outline: Key Elements to NEMO

- NEMO Goal
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- Anticipated / Expected:
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- Unexpected / Breakthroughs:
  - Treatment of extended ...
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, ... warping, indirect gaps
- Putting it all together
  - NEMO - testmatrix
  - The next step: automated analysis and SYNTHESIS

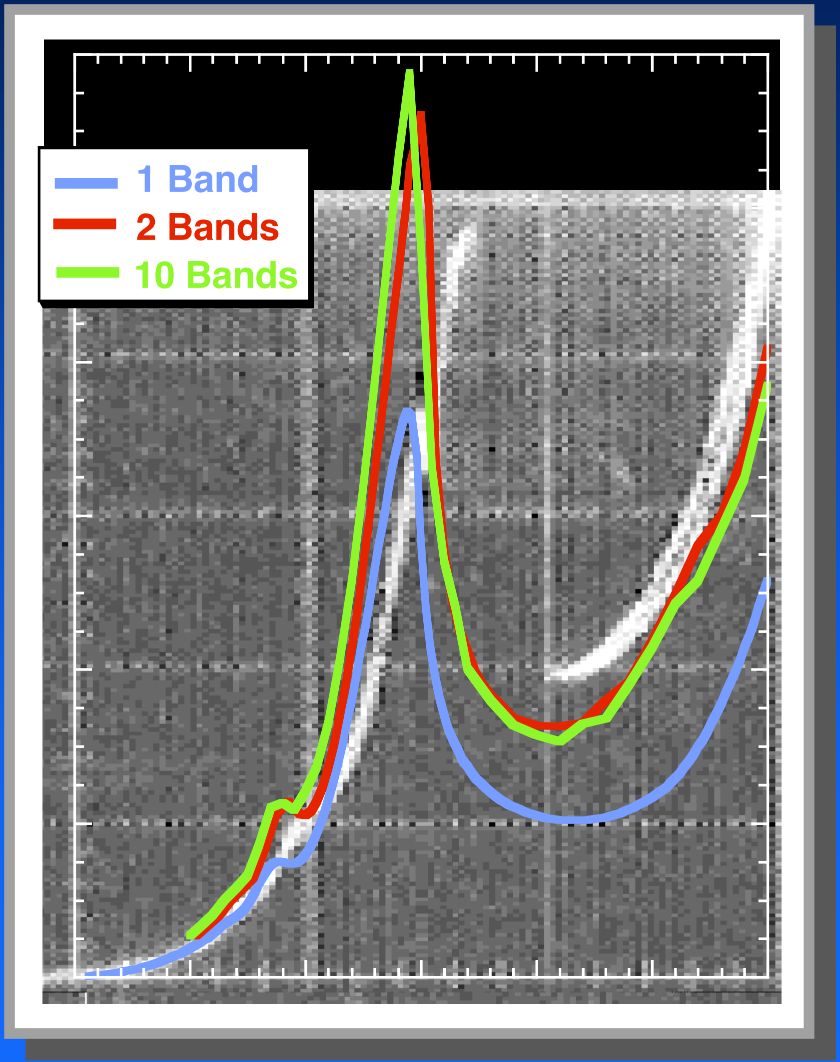
•Unexpected / Breakthroughs:

•Full bandstructure
Non-parabolicity
band warping
indirect materials



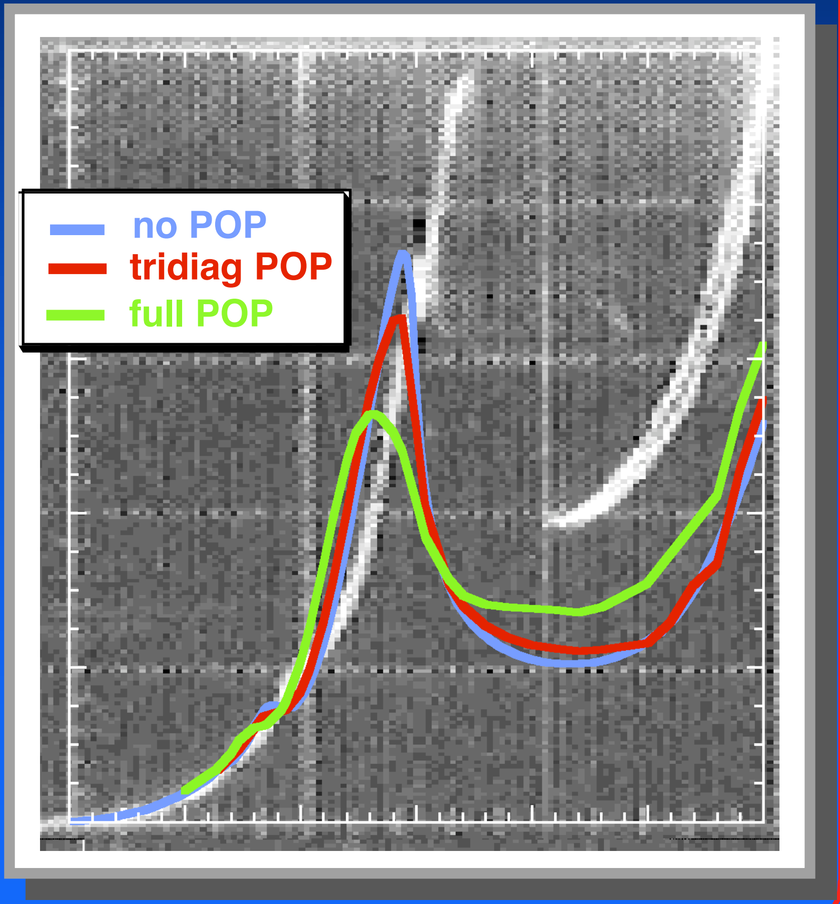
Single Band vs. Multiband

Multiband without scattering

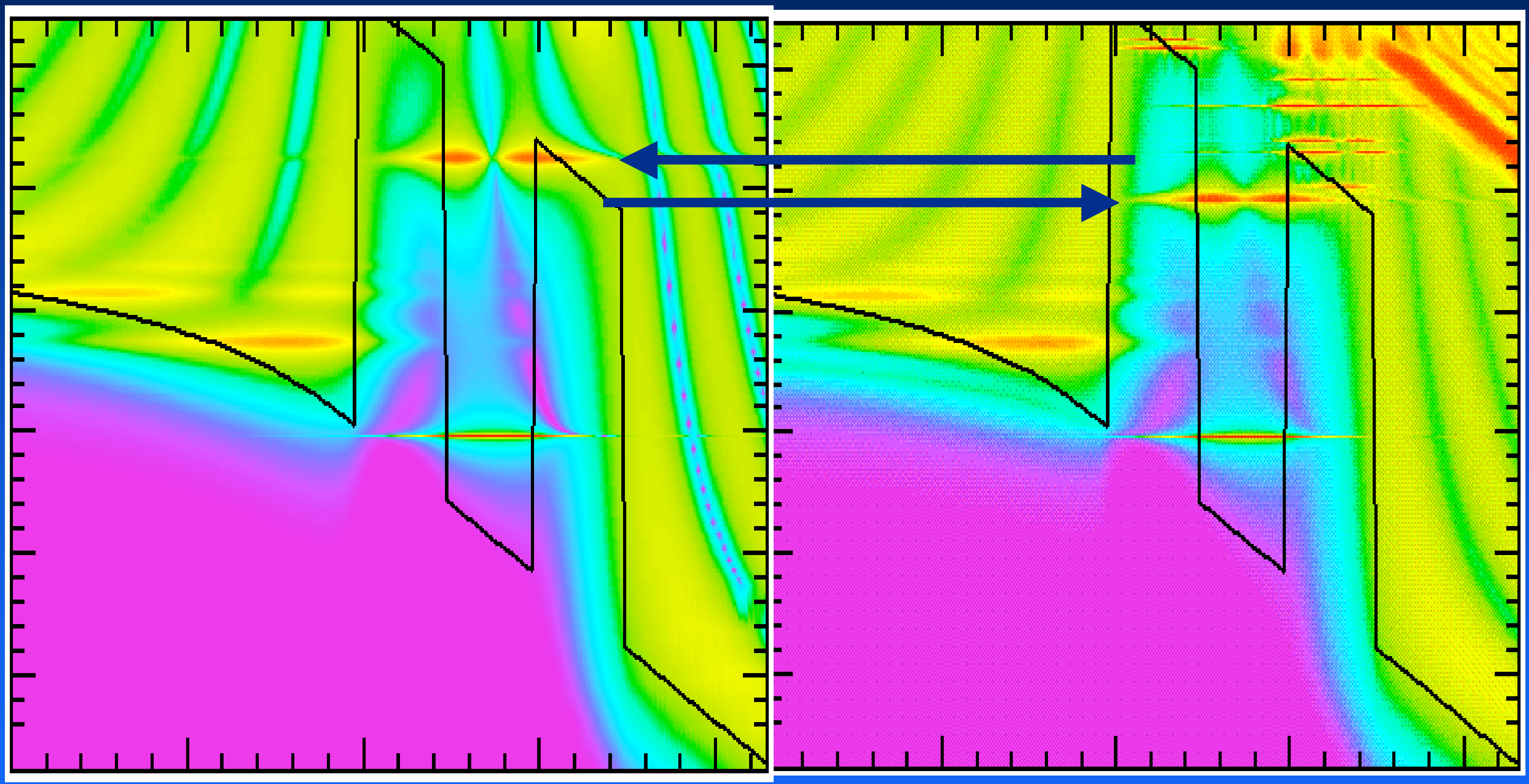


Single band with scattering

POP = Polar Optical Phonons

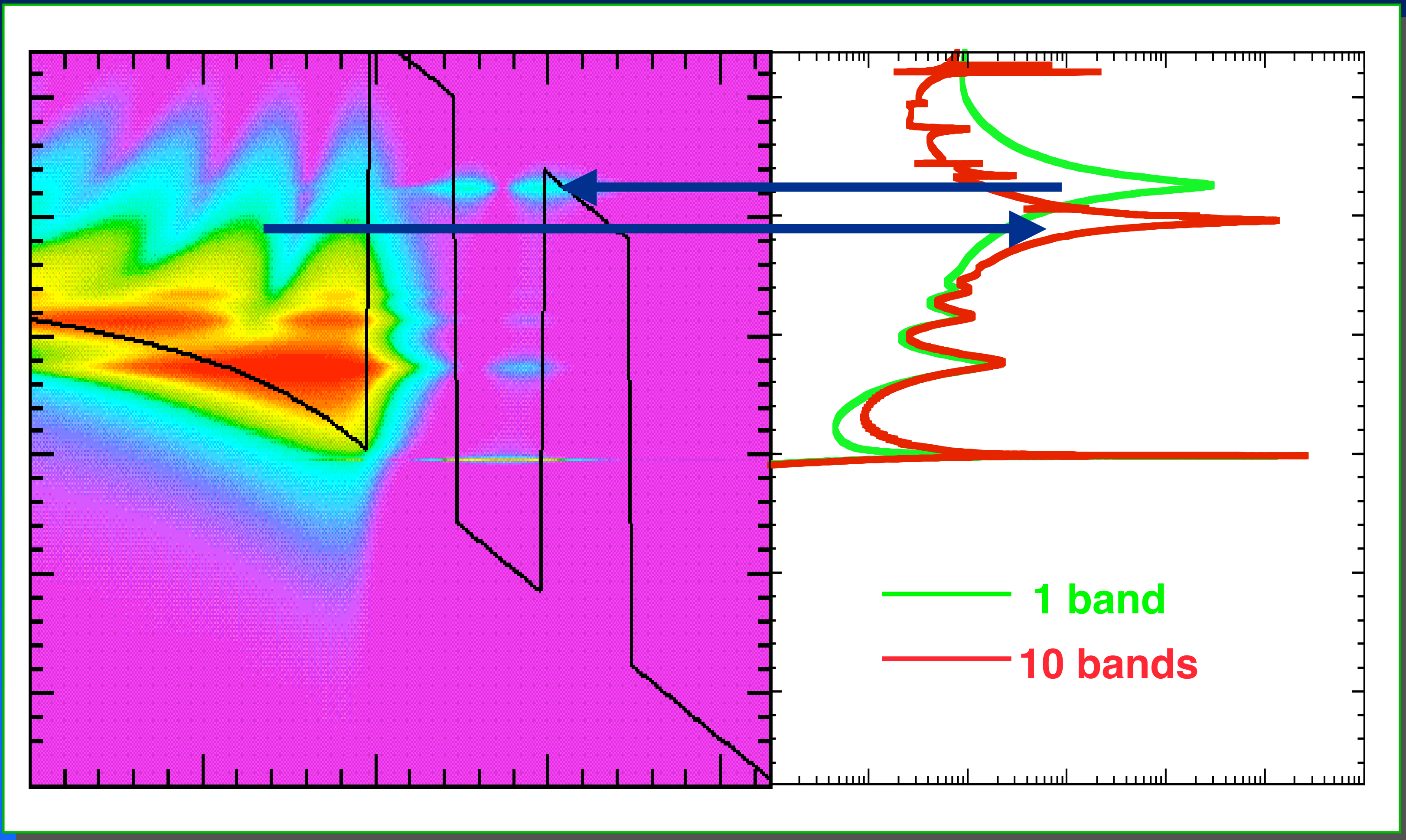


Comparison of 1 and 10 Band Densities of States



10 band lowers 2nd resonance

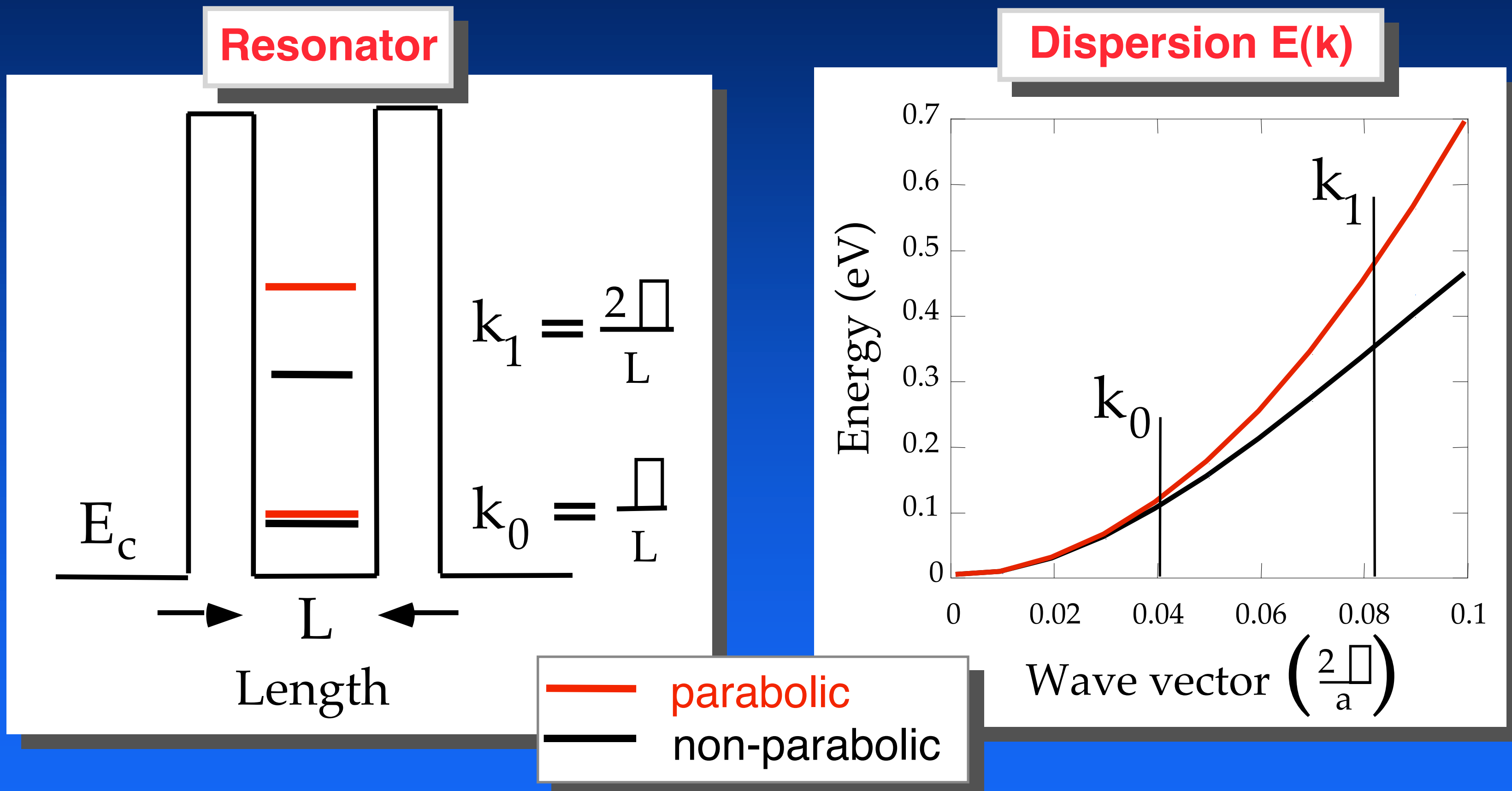
Current Flow through the Second Resonance



1 band electron density

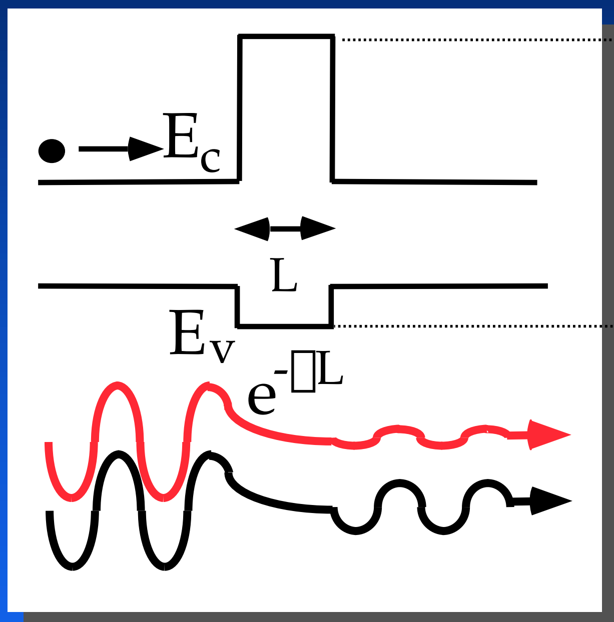
current density

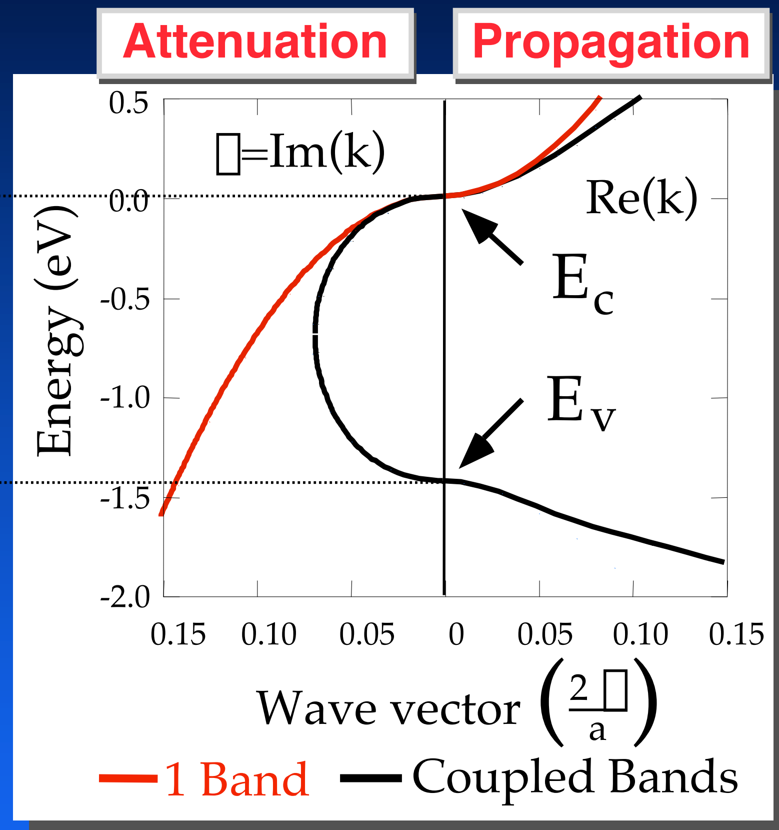
Resonance State Lowering due to Band Non-Parabolicity



Second diode turn-on at lower voltages.

Wave Attenuation in Barriers

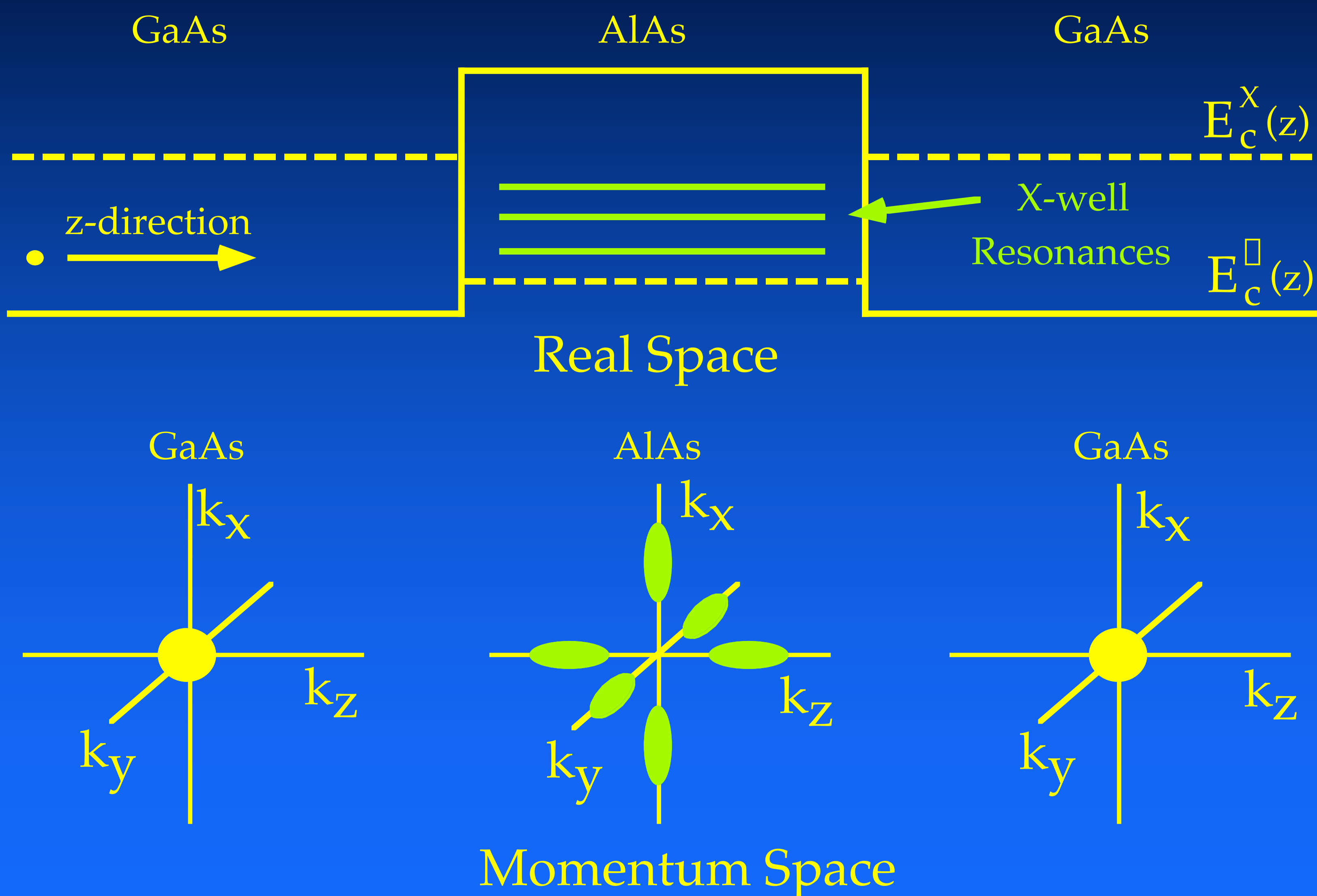




- Attenuation is smaller with coupled bands
- Tunneling probability increases
- Current increases

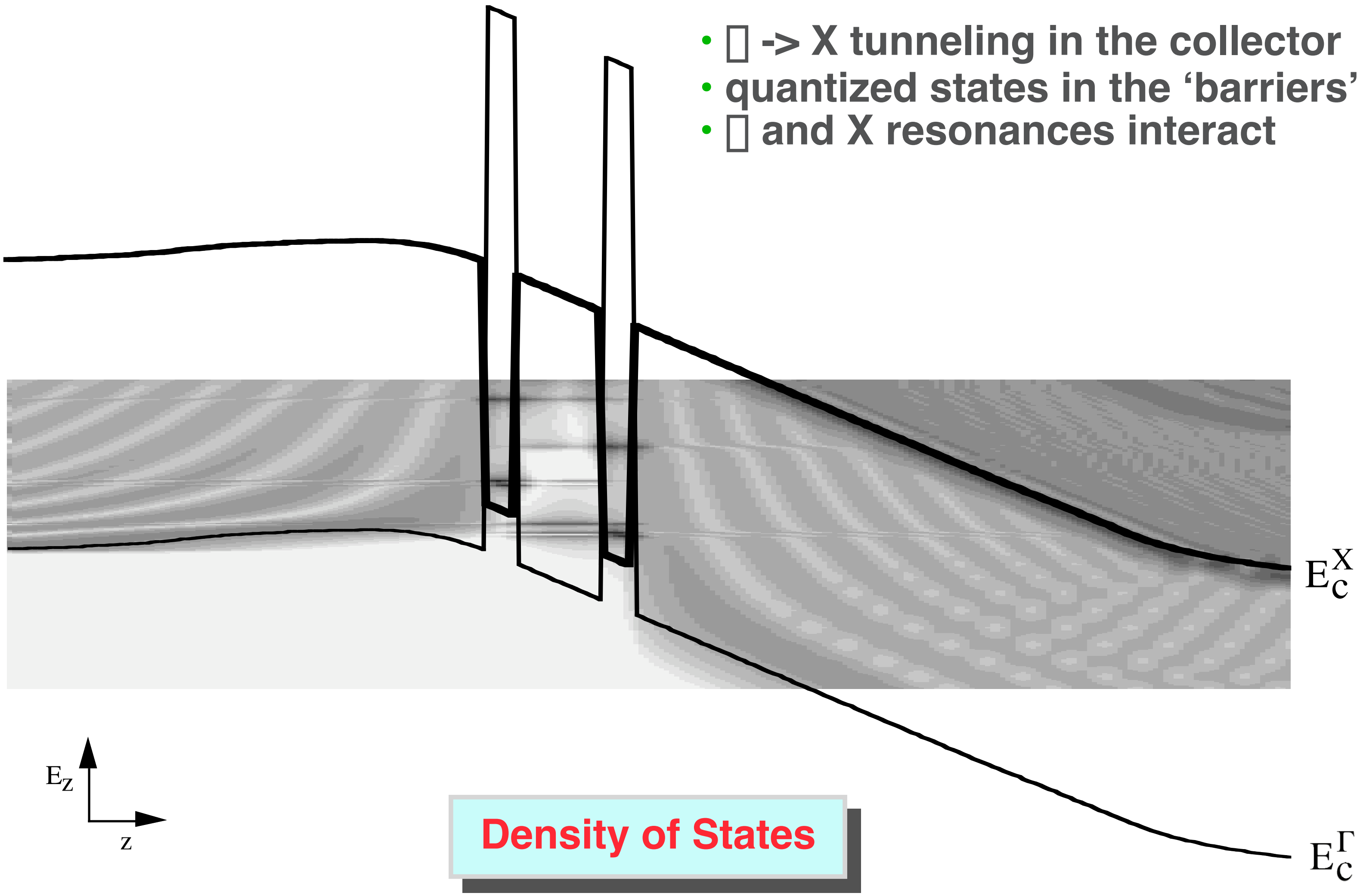
=> Barriers are more transparent than expected!!!

Transport in Indirect Gap Barriers



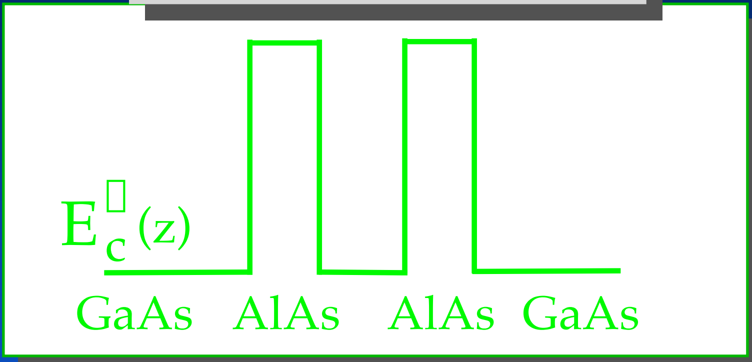
Multiband Effects in GaAs/AlAs RTD’s

- □ -> X tunneling in the collector
- quantized states in the ‘barriers’
- □ and X resonances interact

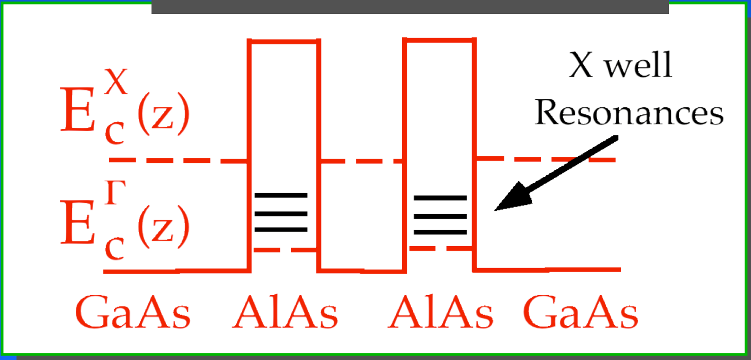


GaAs / AlAs RTD Simulation

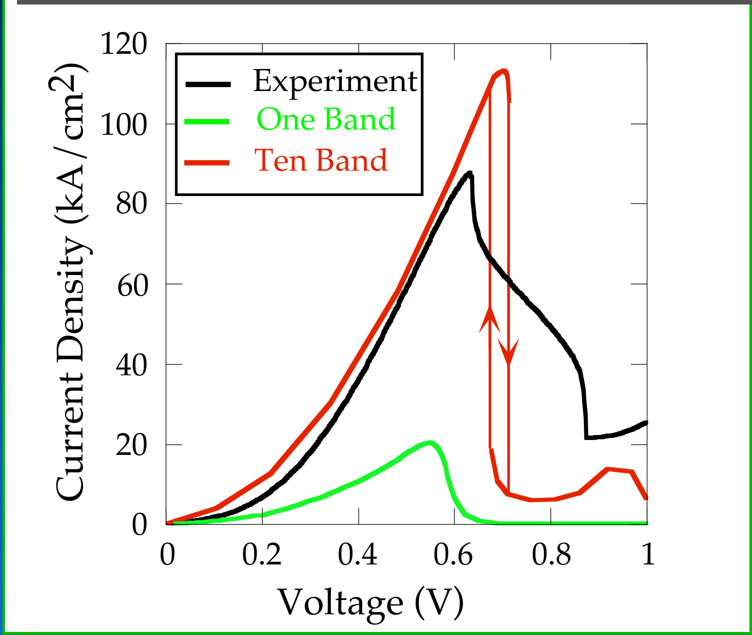
Single Band Model



Multi-Band Model



Current Density vs. Voltage



Agreement between simulation and experiment has significantly improved with the addition of band structure effects.

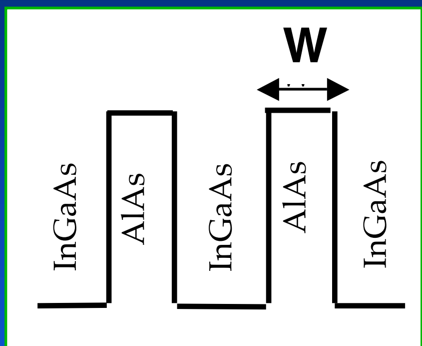
Outline:
Key Elements to NEMO

- **NEMO Goal:**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- **Anticipated / Expected:**
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- **Unexpected / Breakthroughs:**
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, complex band warping, indirect gaps
- **Putting it all together**
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**

Testmatrix-Based Verification (room temperature)

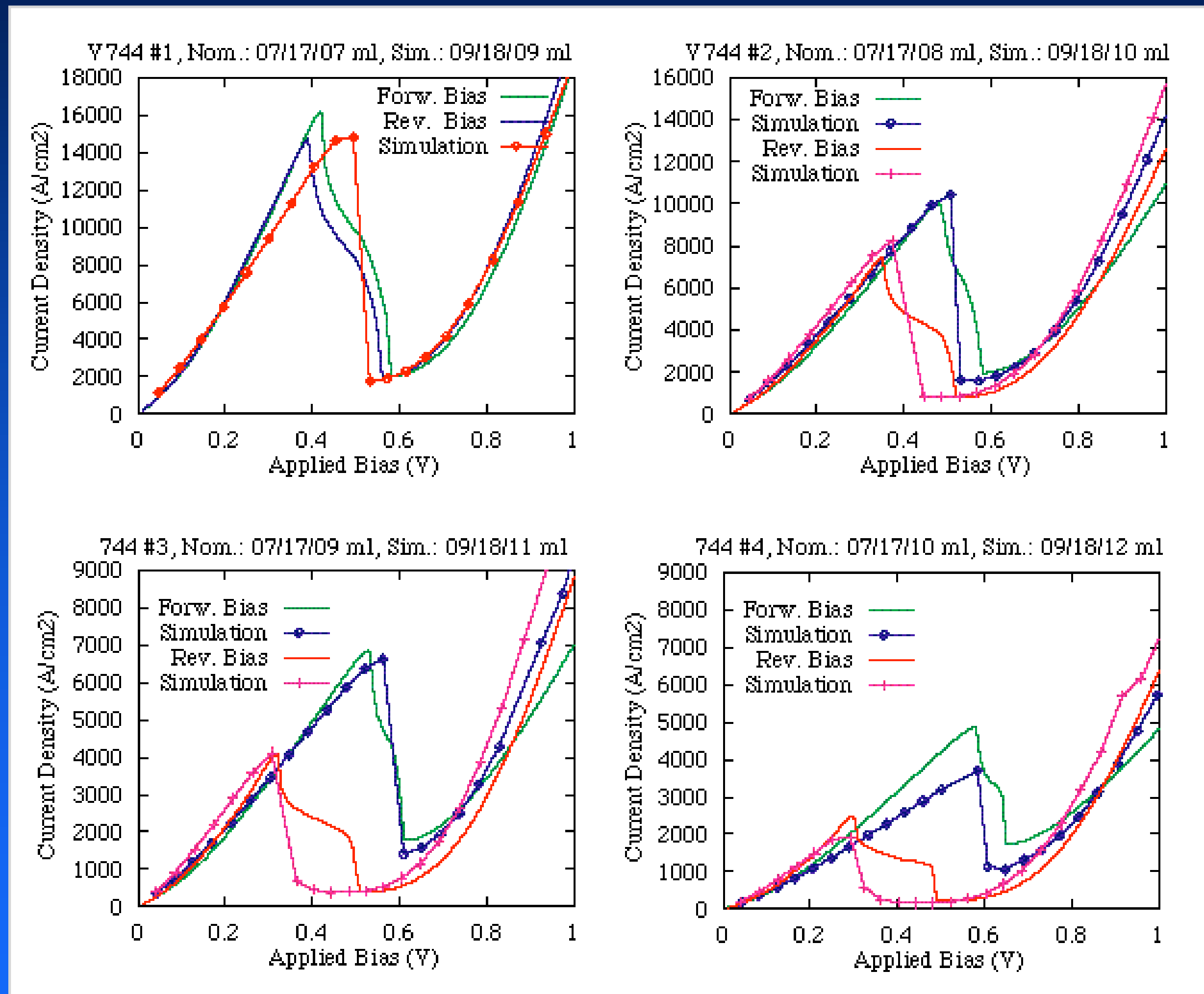
Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

Vary One Barrier Thickness



Four increasingly asymmetric devices:

20/50/20 Angstrom
20/50/23 Angstrom
20/50/25 Angstrom
20/50/27 Angstrom

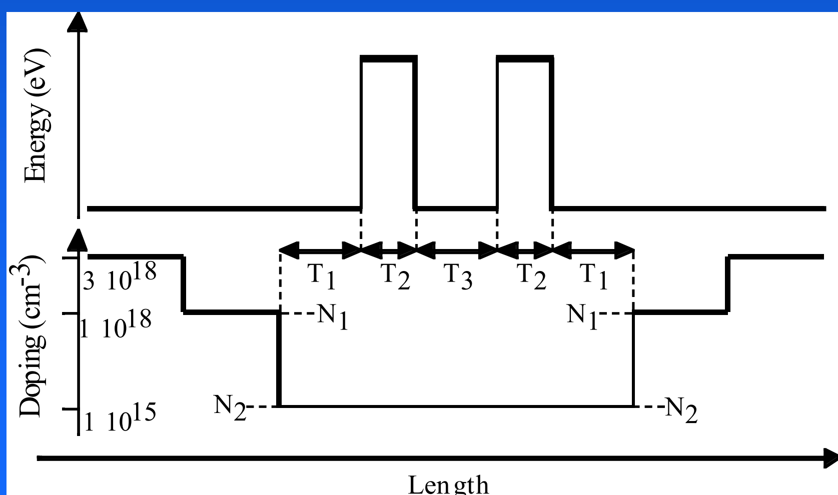


Genetically Engineered Nanoelectronic Structures (GENES)

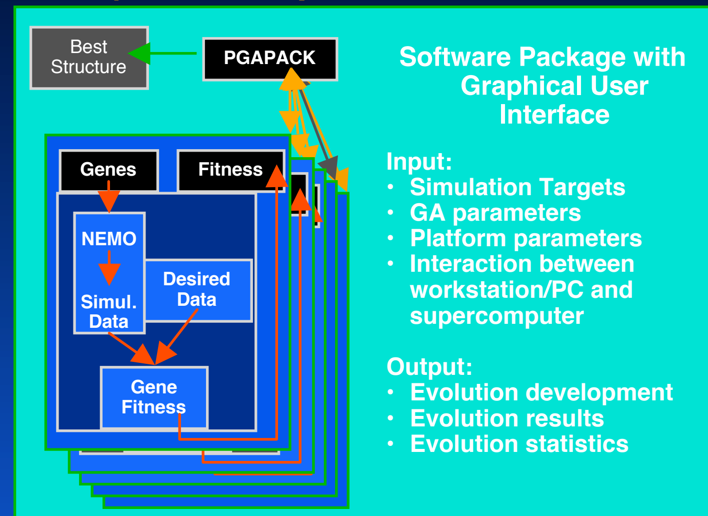
Objectives:
- Automate nanoelectronic device synthesis, analysis, and optimization using genetic algorithms (GA).

Approach:
- Augment parallel genetic algorithm (PGApack).
- Combine PGApack with NEMO.
- Develop graphical user interface for GA.

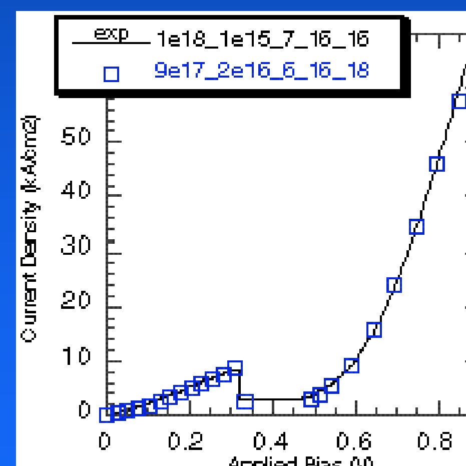
How do you know what you have built?



Architecture



Results:
Nanoelectronic Device Structural analysis



GA analyzed atomic monolayer structure and doping profile of RTD device

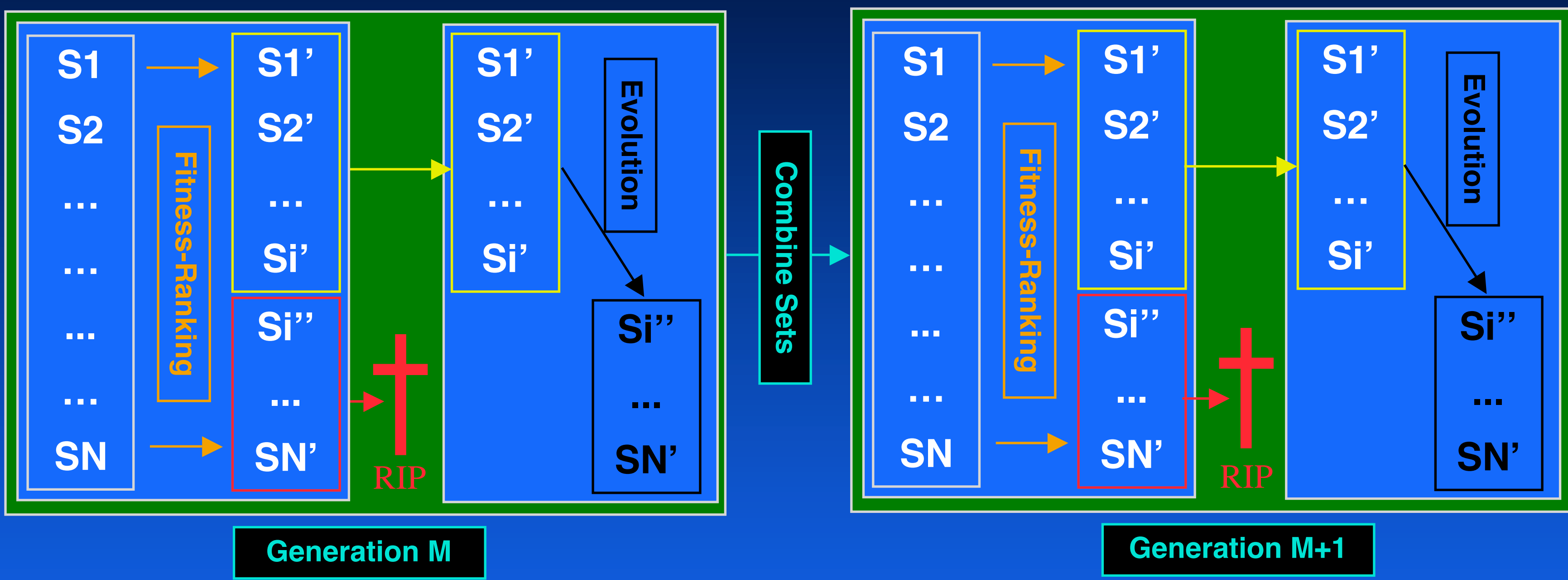
Black: structure specs, Blue: Best fit

Gerhard Klimeck

Key Elements to NEMO Conclusions

- **NEMO Goals Achieved:**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- **Lessons Learned:**
  - Comprehensive theory approach really did work.
  - Needed close coupling to well controlled test matrices.
  - Contact treatment and full bandstructure approach brought breakthrough.
  - Scattering (in central RTD) was not the most important (against all predictions).
    Scattering in the contacts is the most important effect, but we need to fake it through relaxation time approximation.
  - Can perform automated device synthesis and analysis.

Basic Genetic Algorithm



- Genetic algorithm parameter optimization is based on:
  - Survival of good parameter sets
  - Evolution of new parameter sets
  - Survival of a diverse population

- Optimization can be performed globally, rather than locally.

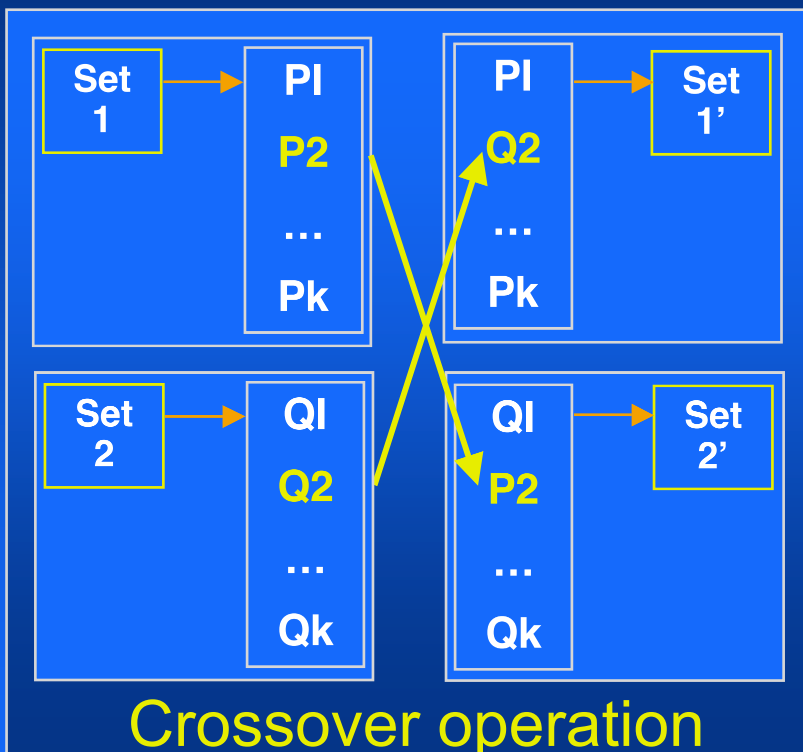
Basic Evolution Operations

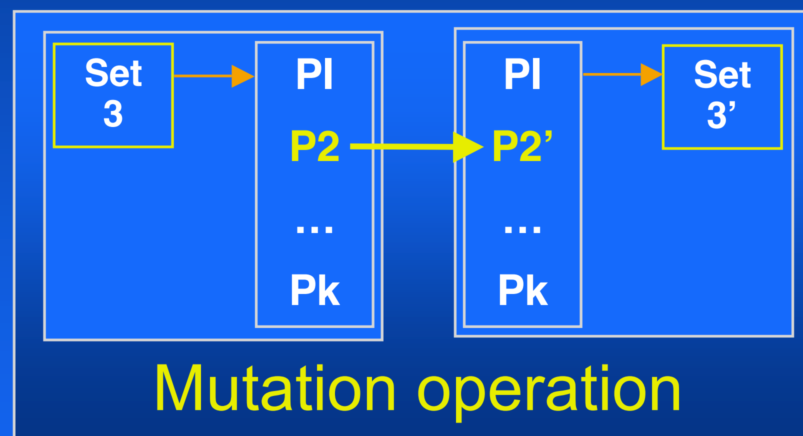
Each set (Si) consists of several parameters (Pj)

The parameters Pj can be of different kinds: real, integers, symbols.....

Gross Exploration

Fine Tuning



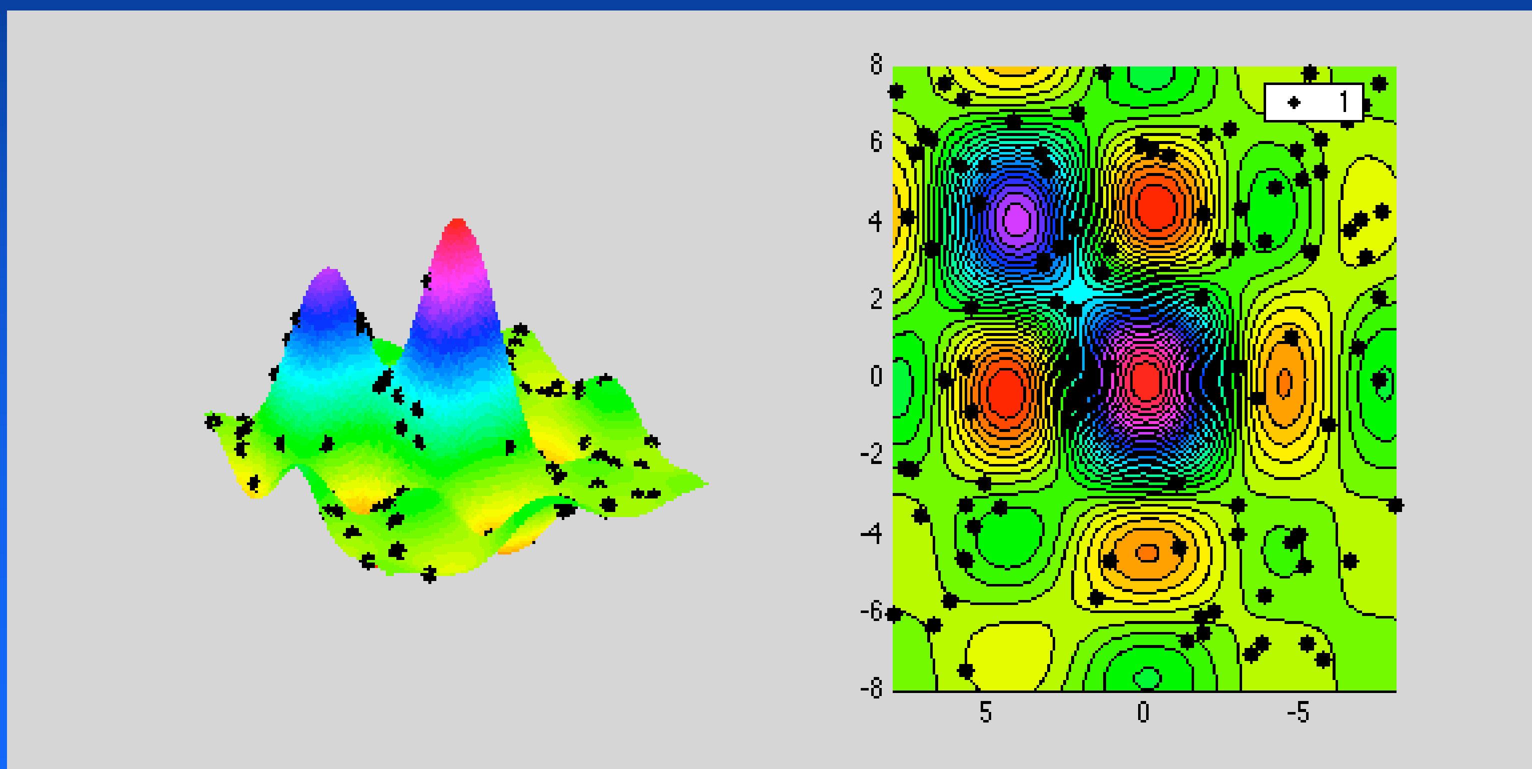


Crossover explores different combinations of existing

- Creation of new gene values.

Global Optimization via Genetic Algorithms

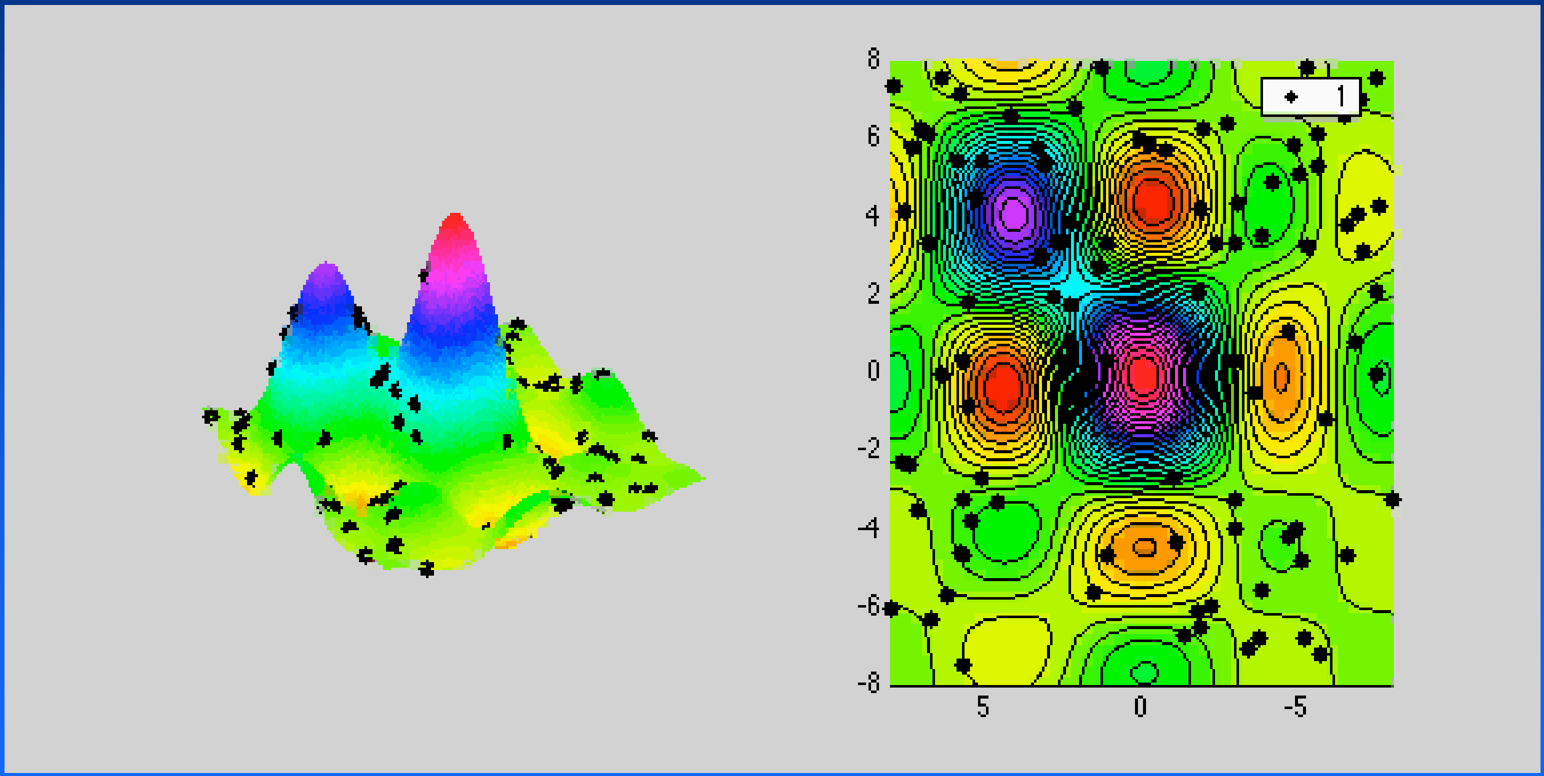
$$F(x,y) = \frac{\sin(x)}{x}\frac{\sin(y)}{y} + 0.7\,\frac{\sin(x-4)}{(x-4)}\frac{\sin(y-4)}{(y-4)}$$



Global Optimization: Genetic Algorithm Development

Genetic Algorithm Convergence

pop = 100, 300 generations, steady-state (10%), 2-point crossover p = 0.85, mutatation p = 1/2



Outline:
Key Elements to NEMO

- **Unexpected / Breakthroughs:**
  - **Treatment of extended contact regions**

- **NEMO Goal**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD’s).
  - Faster simulation than experimental turn-around (1 week).
- **Anticipated / Expected:**
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- **Unexpected / Breakthroughs:**
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, spd5s*
    - Non-parabolicity, complex band warping, indirect gaps
- **Putting it all together**
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**

JPL

Outline:
Key Elements to NEMO

- NEMO Goal:
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- Anticipated / Expected:
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- Unexpected / Breakthroughs:
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, complex band warping, indirect gaps
- Putting it all together
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**

•Unexpected / Breakthroughs:

•Full bandstructure
Non-parabolicity
band warping
indirect materials

Outline:
Key Elements to NEMO

- **NEMO Goal:**
  - Quantitative design and synthesis of resonant tunneling diodes (RTD's).
  - Faster simulation than experimental turn-around (1 week).
- **Anticipated / Expected:**
  - Scattering - origin of the valley current.
  - Charge self-consistency - position of voltage peak.
- **Unexpected / Breakthroughs:**
  - Treatment of extended contact regions
  - Full bandstructure - Empirical tight binding: sp3s*, sp3d5s*
    - Non-parabolicity, complex band warping, indirect gaps
- **Putting it all together**
  - NEMO - testmatrix
  - **The next step: automated analysis and SYNTHESIS**